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A simple rhodium-catalyzed addition reaction of aldehydes with arylboronic acids in aqueous γ-valerolactone

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Contents

General Experimental

Unless otherwise noted, all chemicals were purchased from commercial suppliers (Aladdin) and used without further purification. ^{1}H NMR and ^{13}C NMR spectra were recorded at ambient temperature on a Bruker AVANCE Ⅲ 500 spectrometer (^{1}H: 500 MHz; ^{13}C: 125 MHz). Chemical shifts are reported in δ units, parts per million (ppm), and were referenced to $CDCl_3$ (7.26 or 77.0 ppm) as the internal standard. The coupling constants *J* are given in Hz. Column chromatography was performed using EM Silica gel 60 (300-400 mesh). High-resolution mass spectrometry (HRMS) was performed on an Agilent Q-TOF 6540 MS instrument with an ESI source.

Experimental Procedures, Spectral and Analytical data

General procedure for the synthesis of 3aa-ar

A sealed tube equipped with a magnetic stirrer bar was charged with 4-nitrobenzaldehyde **1a** (0.2 mmol), boronic acid **2a-r** (0.3 mmol, 1.5 equiv), $Rh(PPh_3)_3Cl$ (0.5 mol%), Na_2CO_3 (0.3 mmol, 1.5 equiv) and GVL/H_2O (1:1, 2 mL) under N_2. The reaction mixture was then heated to 110 °C and stirred for 6 h. Upon reaction completion, the resulting solution was quenched with water and extracted with ethyl acetate. The collected organic extracts were dried over Na_2SO_4. The solvent was then removed under reduced pressure and the residue was purified by silica gel column chromatography using petroleum ether/ethyl acetate (10:1) as eluent to afford product **3aa-ar**.

General procedure for the synthesis of 3ba-qa

A sealed tube equipped with a magnetic stirrer bar was charged with aldehyde **1b-q** (0.2 mmol), phenylboronic acid **2a** (0.3 mmol, 1.5 equiv), $Rh(PPh_3)_3Cl$ (1 mol%), Na_2CO_3 (0.3 mmol, 1.5 equiv) and GVL/H_2O (1:1, 2 mL) under N_2. The reaction mixture was then heated to 110 °C and stirred for 12 h. Upon reaction completion, the resulting solution was quenched with water and extracted with ethyl acetate. The collected organic extracts were dried over Na_2SO_4. The solvent was then removed under reduced pressure and the residue was purified by silica gel column chromatography using petroleum ether/ethyl acetate (10:1) as eluent to afford product **3ba-qa**.

Characterization data of products 3aa-ar, 3ba-qa

(4-Nitrophenyl)(phenyl)methanol (**3aa**).[S1] Yellow solid (45 mg, 99%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.16-8.14(m, 2H), 7.55 (d, *J* = 7.5 Hz, 2H), 7.36-7.25 (m, 5H), 5.88 (s, 1H), 2.59 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.8, 147.2, 142.7, 128.9, 128.4, 127.1, 126.7, 123.7, 75.5.

(4-Nitrophenyl)(o-tolyl)methanol (**3ab**).[S2] Yellow oil (48 mg, 99%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.5Hz, 2H), 7.48 (d, *J* = 8.5 Hz, 2H), 7.35-7.13 (m, 4H), 6.05 (s, 1H), 2.68 (s, 1H), 2.28 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.3,147.1, 140.4, 135.6, 131.0, 128.3, 127.5, 127.0, 126.5, 123.6, 72.7, 19.4.

(4-Nitrophenyl)(m-tolyl)methanol (**3ac**).[S3] Yellow solid (48 mg, 99%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14-8.12 (m, 2H), 7.54 (d, *J* = 8.5 Hz, 2H), 7.21-7.25(m, 1H), 7.09-7.12 (m, 3H), 5.83 (s, 1H), 2.73 (s, 1H), 2.32 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.0, 147.1, 142.7, 138.7, 129.1, 128.8, 127.3, 127.0, 123.8, 123.6, 75.5, 21.4.

(4-Nitrophenyl)(p-tolyl)methanol (**3ad**).[S1] Yellow solid (48 mg, 99%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.13-8.10(m, 2H), 7.51 (d, *J* = 8.5 Hz, 2H), 7.16 (dd, *J* = 26.0, 8.0 Hz, 4H), 5.82 (s, 1H), 2.82 (s, 1H), 2.31 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.1, 147.1, 139.9, 138.2, 129.6, 127.0, 126.7, 123.6, 75.3, 21.1.

(4-(tert-Butyl)phenyl)(4-nitrophenyl)methanol (**3ae**).[S4] Yellow solid (54 mg, 95%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.15 (d, *J* = 8.5 Hz, 2H), 7.55 (d, *J* = 8.5 Hz, 2H), 7.36 (d, *J* = 8.5 Hz, 2H), 7.25-7.23 (m, 2H), 5.85 (s, 1H), 2.65 (d, *J* = 2.5Hz, 1H), 1.29 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.5, 151.0, 147.1, 139.8, 127.1, 126.5, 125.9, 123.6, 75.3, 34.6, 31.3.

(4-Nitrophenyl)(4-vinylphenyl)methanol (**3af**). Brown solid (41 mg, 80%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.15 (d, *J* = 9.0 Hz, 2H), 7.54 (d, *J* = 9.0 Hz, 2H), 7.38 (d, *J* = 8.0 Hz, 2H), 7.28 (d, *J* = 8.5 Hz, 2H), 6.68 (dd, *J* = 17.5, 10.5 Hz, 1H), 5.87 (s, 1H), 5.74 (d, *J* = 17.5 Hz, 1H), 5.26 (d, *J* = 10.5 Hz, 1H), 2.67 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.7, 147.2, 142.2, 137.8, 136.1, 127.1, 126.9, 126.7, 123.7, 114.6, 75.3. HRMS m/z (ESI) calcd for $C_{15}H_{14}NO_3$ $(M+H)^+$ 256.0968, found 256.0976.

(4-Chlorophenyl)(4-nitrophenyl)methanol (**3ag**).[S1] Yellow solid (52 mg, 99%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14-8.17 (m, 2H), 7.53 (d, *J* = 8.5 Hz, 2H), 7.33-7.26 (m, 4H), 5.88 (s, 1H), 2.72 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.4, 147.3, 141.2, 134.2, 129.1, 128.0, 127.1, 123.8, 74.8.

(4-Bromophenyl)(4-nitrophenyl)methanol (**3ah**).[S5] Yellow solid (46 mg, 76%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.21-8.18 (m, 2H), 7.48-7.56(m, 4H), 7.24-7.22 (m, 2H), 5.89 (s, 1H), 2.41 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.1, 147.4, 141.6, 132.1, 128.4, 127.1, 123.8, 122.4, 74.9.

(4-Fluorophenyl)(4-nitrophenyl)methanol (**3ai**).[S1] Yellow solid (46 mg, 93%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.16 (d, *J* = 9.0 Hz, 2H), 7.54 (d, *J* = 9.0 Hz, 2H), 7.32-7.28 (m, 2H), 7.05-7.01 (m, 2H), 5.89 (s, 1H), 2.75 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.5 (d, $J_{C\text{-}F}$ = 245.8 Hz), 150.7, 147.2, 138.6(d, $J_{C\text{-}F}$ = 3.3 Hz),128.5(d, $J_{C\text{-}F}$ = 8.9 Hz), 127.1, 123.7, 115.8(d, $J_{C\text{-}F}$ = 20.9 Hz), 74.8.

(4-Nitrophenyl)(4-(trifluoromethyl)phenyl)methanol (**3aj**).[S6] Yellow solid (43 mg, 73%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.5 Hz, 2H), 7.61 (d, *J* = 8.5 Hz, 2H), 7.55(d, *J* = 9.0 Hz, 2H), 7.49 (d, *J* = 8.0 Hz, 2H),.5.97 (s, 1H), 2.83 (d, *J* = 23.5 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.0, 147.4, 146.4, 130.4 (q, $J_{C\text{-}F}$ = 3.2 Hz), 127.2, 126.9, 125.8(q, $J_{C\text{-}F}$ = 3.7 Hz), 123.9, 123.8 (d, $J_{C\text{-}F}$ = 270.5 Hz), 74.9.

(4-Methoxyphenyl)(4-nitrophenyl)methanol (**2ak**).[S1] Yellow solid (49 mg, 95%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.5 Hz, 2H), 7.52 (d, *J* = 8.5 Hz, 2H), 7.21 (d, *J* = 8.5 Hz, 2H), 6.85 (d, *J* = 8.5 Hz, 2H), 5.82 (s, 1H), 3.76 (s, 3H), 2.82 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.6, 151.2, 147.1, 135.1, 128.1, 127.0, 123.6,

114.3, 75.0, 55.3.

(4-Nitrophenyl)(4-phenoxyphenyl)methanol (**3al**). Yellow solid (51 mg, 80%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.22-8.19 (m, 2H), 7.58 (d, *J* = 8.5 Hz, 2H), 7.35-7.27 (m, 4H), 7.12 (t, *J* = 7.5 Hz, 1H), 7.01-6.97 (m, 4H), 5.94 (s, 1H), 2.35(d, *J* =2.5 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.6, 156.7, 150.7, 147.3, 137.4, 129.9, 128.3, 127.0, 123.7, 119.2, 118.9, 75.1. HRMS m/z (ESI) calcd for $C_{19}H_{16}NO_4$ $(M+H)^+$ 322.1074, found 322.1088.

(4-(Benzyloxy)phenyl)(4-nitrophenyl)methanol (**3am**). Yellow solid (60 mg, 90%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.19-8.16 (m, 2H), 7.56 (d, *J* = 8.5 Hz, 2H), 7.42-7.30 (m, 5H), 7.26-7.22 (m, ,3H), 6.97-6.93 (m, 2H), 5.87 (s, 1H), 5.05 (s, 2H), 2.28 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.9, 151.0, 147.2, 136.7, 135.3, 128.6, 128.2, 128.1, 127.4, 127.0, 123.7, 115.3, 75.1, 70.1. HRMS m/z (ESI) calcd for $C_{20}H_{18}NO_4$ $(M+H)^+$ 336.1230, found 336.1242.

4-(Hydroxy(4-nitrophenyl)methyl)benzonitrile (**3an**).[S7] Yellow solid (28 mg, 55%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.23-8.17 (m, 2H), 7.64 (d, *J* = 8.5 Hz, 2H), 7.57-7.48 (m, 4H), 5.97 (s, 1H), 2.85 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.6, 147.6, 132.7, 127.2, 127.0, 124.0, 123.7, 118.4, 112.1, 74.8.

4-(Hydroxy(4-nitrophenyl)methyl)benzaldehyde (**3ao**).[S8] Yellow solid (23 mg, 45%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.86 (s, 1H), 8.10-8.08 (m, 2H), 7.75 (d, *J* = 8.0 Hz, 2H), 7.49-7.42 (m, 4H), 5.91 (s, 1H), 3.11 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 191.9, 150.0, 149.2, 147.4, 136.0, 130.3, 127.2, 127.1, 123.9, 75.0.

Ethyl 4-(hydroxy(4-nitrophenyl)methyl)benzoate (**3ap**).[S7] Yellow solid (48 mg, 80%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.15 (d, *J* = 9.0 Hz, 2H), 7.97 (d, *J* = 8.0 Hz, 2H), 7.54 (d, *J* = 9.0 Hz, 2H), 7.42 (d, *J* = 8.0 Hz, 2H), 7.27 (s, 1H), 5.95 (s, 1H), 4.34 (q, *J* = 7.5 Hz, 2H), 3.22 (s, 1H), 1.37 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.3, 150.3, 147.5, 147.3, 130.2, 130.1, 127.2, 126.5, 123.8, 75.0, 61.2, 14.3.

[1,1'-Biphenyl]-4-yl(4-nitrophenyl)methanol (**3aq**).[S1] Yellow solid (60 mg, 99%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.15 (d, *J* = 9.0 Hz, 2H), 7.57-7.53 (m, 6H), 7.43-7.22 (m, 5H), 5.90 (s, 1H), 2.70 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.8, 147.2, 141.7, 141.3, 140.4, 128.9, 127.6, 127.6, 127.2, 127.1, 127.1, 123.7, 75.3.

Naphthalen-1-yl(4-nitrophenyl)methanol (**3ar**).[S1] Yellow oil (53 mg, 95%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.11 (d, *J* = 8.5 Hz, 2H), 7.99 (d, *J* = 8.0 Hz, 1H), 7.90-7.82 (m, 2H), 7.54 (d, *J* = 8.5 Hz, 2H), 7.50-7.42(m, 4H), 6.51 (s, 1H), 2.79 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.4, 147.2, 137.8, 134.2, 130.5, 129.4, 129.0, 127.5, 126.6, 126.0, 125.6, 125.3, 123.8, 123.6, 73.3.

Diphenylmethanol (**3ba**).[S1] White solid (35 mg, 95%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40-7.36 (m, 4H), 7.35-7.31 (m, 4H), 7.28-7.24 (m, 2H), 5.84 (s, 1H), 2.25 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 143.8, 128.5, 127.6, 126.6, 76.3.

(4-Methoxyphenyl)(phenyl)methanol (**3ca**).[S9] Colorless oil (38 mg, 90%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36-7.29(m, 4H), 7.26-7.22 (m, 3H), 6.86-6.83 (m, 2H), 5.75 (s, 1H), 3.76 (s, 3H), 2.35 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.0, 144.1, 136.2, 128.4, 127.9, 127.4, 126.4, 113.9, 75.8, 55.3.

[1,1'-Biphenyl]-4-yl(phenyl)methanol (**3da**).[S10] Yellow solid (48 mg, 93%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53 (t, *J* = 8.0 Hz, 4H), 7.41-7.36 (m, 6H), 7.29-7.33 (m, 3H), 7.25 (t, *J* = 7.5Hz, 1H), 5.80 (s, 1H), 2.52 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 143.9, 142.9, 140.9, 140.5, 128.8, 128.6, 127.7, 127.4, 127.3, 127.2, 127.1, 126.7, 76.1.

(4-Fluorophenyl)(phenyl)methanol (**3ea**).[S9] Colorless oil (36 mg, 90%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38-7.25 (m, 7H), 7.01-6.98 (m, 2H), 5.79 (s, 1H), 2.36 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.2 (d, J_{C-F}

=244.4Hz), 143.7, 139.6(d, J_{C-F} =3.0Hz), 128.6, 128.3(d, J_{C-F} =8.0Hz), 127.7, 126.5, 115.3(d, J_{C-F} =21.4 Hz), 75.6.

Phenyl(4-(trifluoromethyl)phenyl)methanol (**3fa**).[S9] Yellow solid (47 mg, 95%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.0 Hz, 2H), 7.51 (d, *J* = 8.0 Hz, 2H), 7.36-7.25 (m, 5H), 5.87 (s, 1H), 2.37 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 147.6, 143.2, 129.7（q, J_{C-F} = 32.5 Hz）, 128.9, 128.1, 126.7 (d, J_{C-F} = 4.6 Hz), 125.4(q, J_{C-F} =3.7 Hz), 125.2, 123.1, 75.8.

4-(Hydroxy(phenyl)methyl)benzonitrile (**3ga**).[S1] Colorless oil (41 mg, 99%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 (d, *J* = 8.0 Hz, 2H), 7.47 (d, *J* = 8.5 Hz, 2H), 7.35-7.26 (m, 5H), 5.81 (s, 1H), 2.87 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.0, 142.8, 132.2, 128.8, 128.2, 127.0, 126.7, 118.8, 111.0, 75.5.

(2-Nitrophenyl)(phenyl)methanol (**3ha**).[S1] Yellow oil (43 mg, 95%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.0 Hz, 1H), 7.74-7.71 (m, 1H), 7.60 (t, *J* = 7.5 Hz, 1H), 7.42 (t, *J* = 8.0 Hz, 1H), 7.33-7.24 (m, 5H), 6.39 (s, 1H), 3.05 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 148.4, 141.6, 138.5, 133.4, 129.4, 128.6, 128.5, 128.0, 127.0, 125.0, 71.5.

(3-Nitrophenyl)(phenyl)methanol (**3ia**).[S1] Yellow oil (44 mg, 96%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.16 (s, 1H), 8.00-7.95 (m, 1H), 7.58 (d, *J* = 7.5 Hz, 1H), 7.36 (t, *J* = 8.0 Hz, 1H), 7.26-7.15 (m, 5H), 5.76 (s, 1H), 2.79 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 148.4, 145.9, 142.8, 132.5, 129.4, 128.9, 128.3, 126.7, 122.4, 121.3, 75.3.

4-(Hydroxy(phenyl)methyl)benzaldehyde (**3ja**).[S1] Yellow oil (17 mg, 40%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.96 (s, 1H), 7.83 (d, *J* = 8.5 Hz, 2H), 7.60 (d, *J* = 8.5 Hz, 2H), 7.36-7.26 (m, 5H), 5.89 (s, 1H), 2.55 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.0, 150.4, 143.1, 135.6, 130.0, 128.8, 128.1, 126.9, 126.7, 75.9.

Methyl 4-(hydroxy(phenyl)methyl)benzoate (**3ka**).[S9] Colorless oil (46 mg, 95%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.95 (d, *J* = 7.5 Hz, 2H), 7.42 (d, *J* = 8.0 Hz, 2H), 7.31-7.30 (m, 5H), 5.81 (s, 1H), 3.85 (s, 3H), 2.84 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.0, 148.9, 143.4, 129.8, 128.7, 128.5, 127.9, 126.7, 126.4, 75.9, 52.1.

(4-(Dimethylamino)phenyl)(phenyl)methanol (**3la**).[S11] Yellow solid (14 mg, 30%). m.p. 69-70 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 (d, *J* = 7.5 Hz, 2H), 7.32 (t, *J* = 7.0 Hz, 2H), 7.25-7.19 (m, 3H), 7.00-6.67 (m, 2H), 5.77 (s, 1H), 2.92 (s, 6H), 2.15 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.2, 144.3, 132.0, 128.3, 127.8, 127.2, 126.4, 112.6, 76.0, 40.6.

Naphthalen-1-yl(phenyl)methanol (**3ma**).[S1] Yellow oil (42 mg, 90%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.0 Hz, 1H), 7.83 (dd, *J* = 23.4, 7.8 Hz, 2H), 7.63 (d, *J* = 7.1 Hz, 1H), 7.49 (t, J = 7.3 Hz, 1H), 7.45 (t, 2H), 7.42 (d, *J* = 7.3 Hz, 2H), 7.33 (t, *J* = 7.3 Hz, 2H), 7.28 (t, *J* = 7.5 Hz, 1H), 6.53 (s, 1H), 2.37 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 143.2, 138.8, 134.0, 130.7, 128.8, 128.5, 128.5, 127.7, 127.0, 126.2, 125.6, 125.3, 124.7, 124.0, 73.7.

Phenyl(thiophen-2-yl)methanol (**3na**).[S1] Yellow oil (19 mg, 50%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 (d, *J* = 7.5 Hz, 2H), 7.34 (t, *J* = 7.5 Hz, 2H), 7.29 (d, *J* = 7.5 Hz, 1H), 7.23-7.21 (m, 1H), 6.92-6.90(m, 1H), 6.85 (d, *J* =1.0 Hz, 1H), 2.62 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 148.2, 143.2, 128.6, 128.0, 126.7, 126.4, 125.4, 124.9, 72.4.

1,2-Diphenylethan-1-ol (**3oa**).[S12] Colourless oil (34 mg, 85%). δ 7.38-7.26 (m, 7H), 7.25-7.15 (m, 3H), 4.90 (dd, *J* = 8.6, 4.6 Hz, 1H), 3.08-2.97 (m, 2H), 1.98 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 143.9, 138.2, 129.5, 128.5, 128.4, 127.6, 126.6, 126.0, 75.4, 46.2.

1-Phenylhexan-1-ol (**3pa**).[S13] Colourless oil (28 mg, 77%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41-7.37 (m, 4H), 7.33-7.30 (m, 1H), 4.71-7.66 (m, 1H), 1.88-1.74 (m, 3H), 1.56-1.33 (m, 6H), 0.90 (t, *J* = 7.0 Hz, 3H). ^{13}C

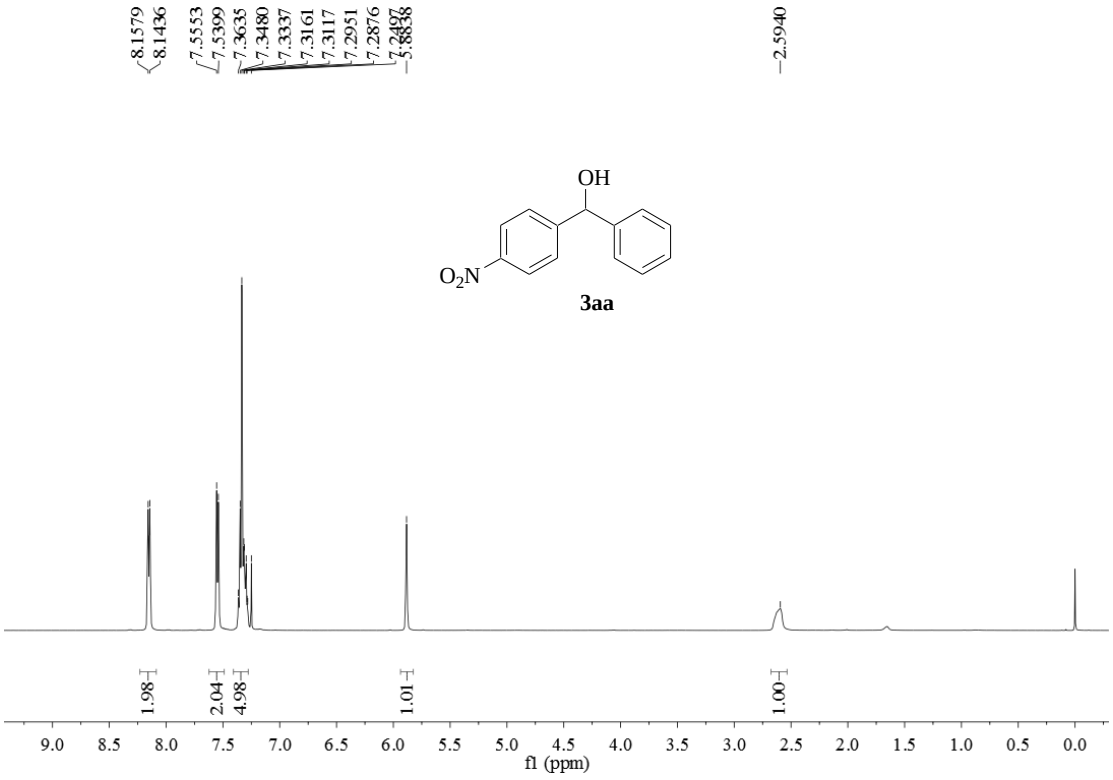
NMR (125 MHz, $CDCl_3$) δ 144.9, 128.4, 127.5, 125.9, 74.7, 39.1, 31.7, 25.5, 22.6, 14.0.

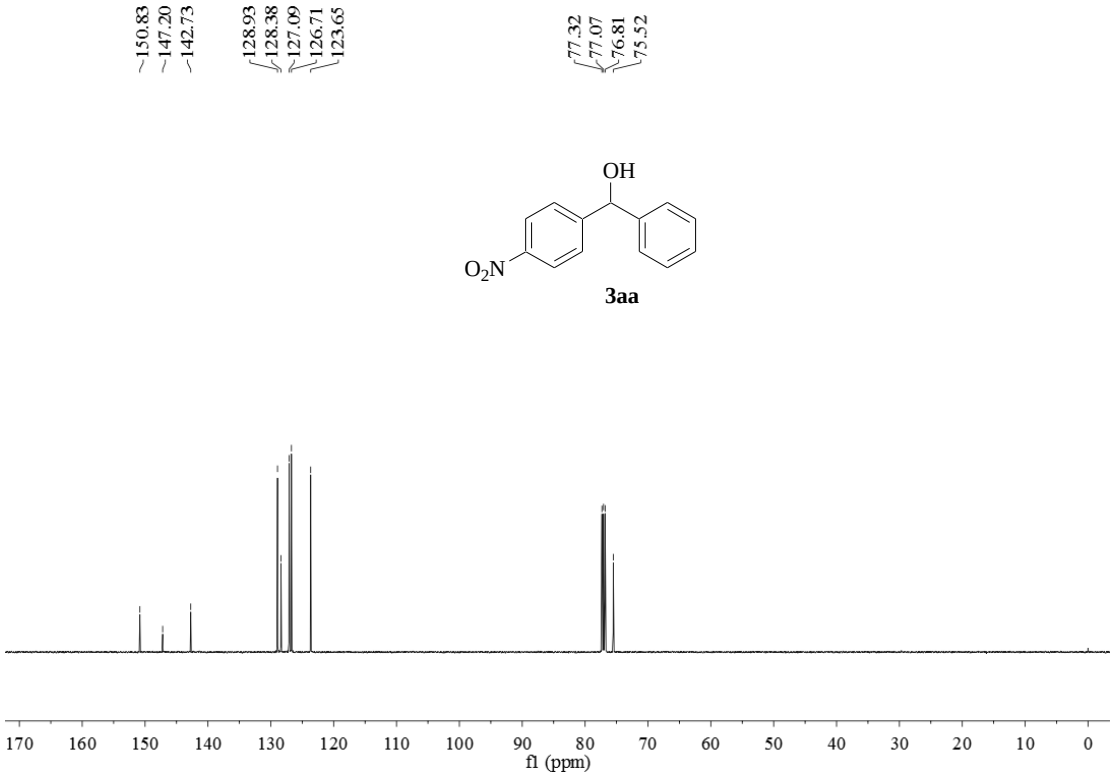
2,2-Dimethyl-1-phenylpropan-1-ol (**3qa**).[S14] Colourless oil (24 mg, 72%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34-7.30 (m, 4H), 7.29-7.25 (m, 1H), 4.41 (d, *J* = 3.0 Hz, 1H), 1.84 (d, *J* = 3.0 Hz, 1H), 0.93 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 142.2, 127.6, 127.5, 127.2, 82.4, 35.6, 25.9.

References

S1. K. Hu, P. Ye, Q. Zhen, X. Yao, T. Xu, Y. Shao, J. Chen, *Molecules*, 2017, **22**, 1580.
S2. J. H. Hall, F. E. Behr, R. L. Reed, *J. Am. Chem. Soc.*, 1972, **94**, 4952.
S3. T. Zou, S.-S. Pi, J.-H. Li, *Org. Lett.*, 2009, **11**, 453.
S4. K. G. Rutherford, O. A. Mamer, *J. Org. Chem.*, 1966, **31**, 2708.
S5. Y.Ogawa, A. Saiga, M. Mori, T. Shibata, K.Takagi, *J. Org. Chem.*, 2000, **65**, 1031.
S6. H. Zhao, M. Cheng, T. Zhang, M. Cai, *J. Organometallic Chem.*, 2015, **777**, 50.
S7. A. Nagaki, K. Imai, S. Ishiuchi, J. Yoshida, *Angew. Chem., Int. Ed.*, 2015, **54**, 1914.
S8. A. Nagaki, H. Yamashita, Y. Takahashi, S. Ishiuchi, K. Imai, J. Yoshida, *Chem. Lett.*, 2018, **47**, 71.
S9. S. Ishida, H. Suzuki, S. Uchida, E. Yamaguchi, A. Itoh, *Eur. J. Org. Chem.*, 2019, 7483.
S10. S. Lin, Y. Liu, S. Peng, S. Liu, *Organometallics* 2020, **39**, 123.
S11. V. Balakrishnan, V. Murugesan, B. Chindan, R. Rasappan, *Org. Lett.*, 2021, **23**, 1333.
S12. C. Zhou, Z. Wang, *Synthesis*, 2005, **10**, 1649.
S13. T. Yamakawa, H. Kinoshita, K. Miura, *J. Organomet. Chem.*, 2013, **724**, 129.
S14. M. Ueno, C. Hori, K. Suzawa, M. Ebisawa, Y. Kondo, *Eur. J. Org. Chem.*, 2005, 1965.

Copies of ^{1}H and ^{13}C NMR Spectra

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O2N
3aa
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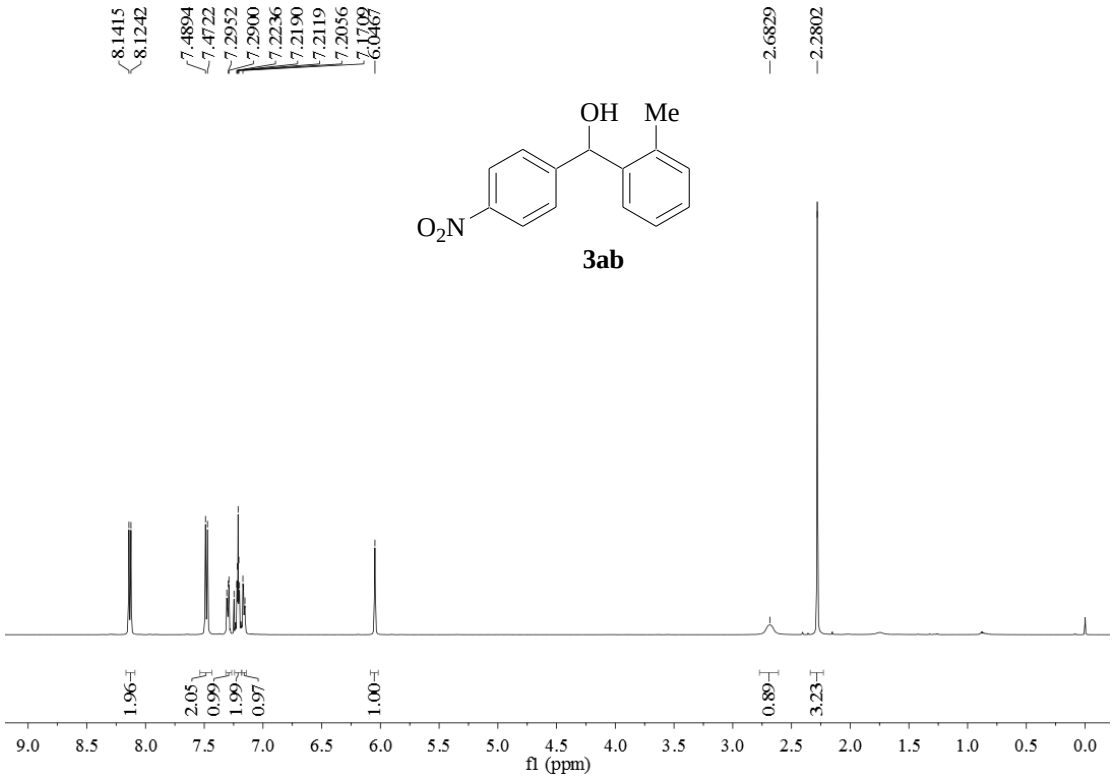
f1 (ppm)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7.1709
6.0467
2.6829
2.2802
OH
Me
O2N
3ab
1.96
2.05
0.99
1.99
0.97
1.00
0.89
3.23
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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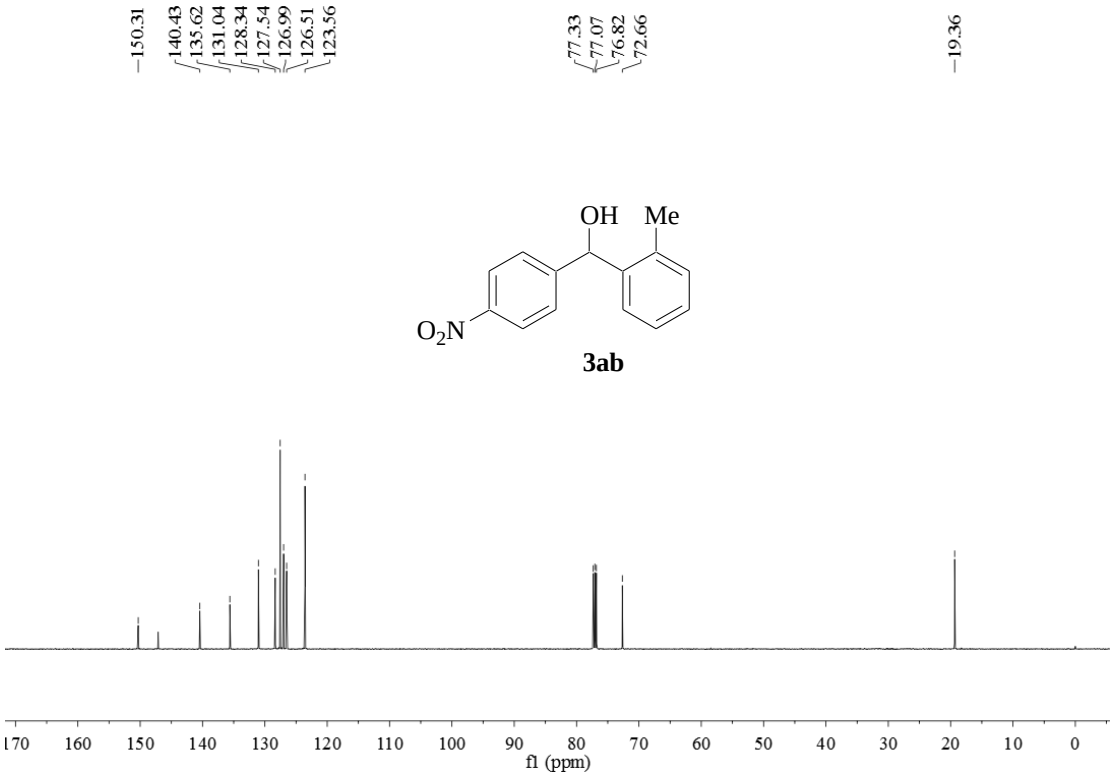
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Me
O2N
3ab
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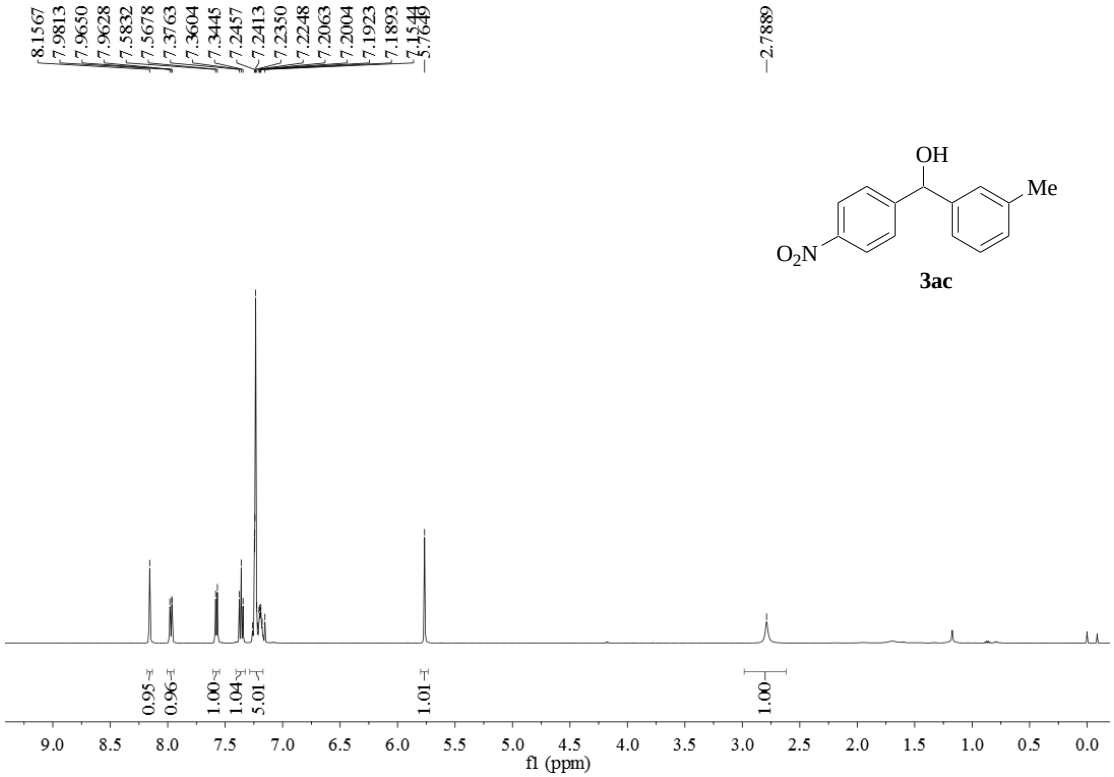
f1 (ppm)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7.2248
7.2063
7.2004
7.1923
7.1893
7.1544
5.7640
2.7889
OH
Me
O2N
3ac
0.95
0.96
1.00
1.04
5.01
1.01
1.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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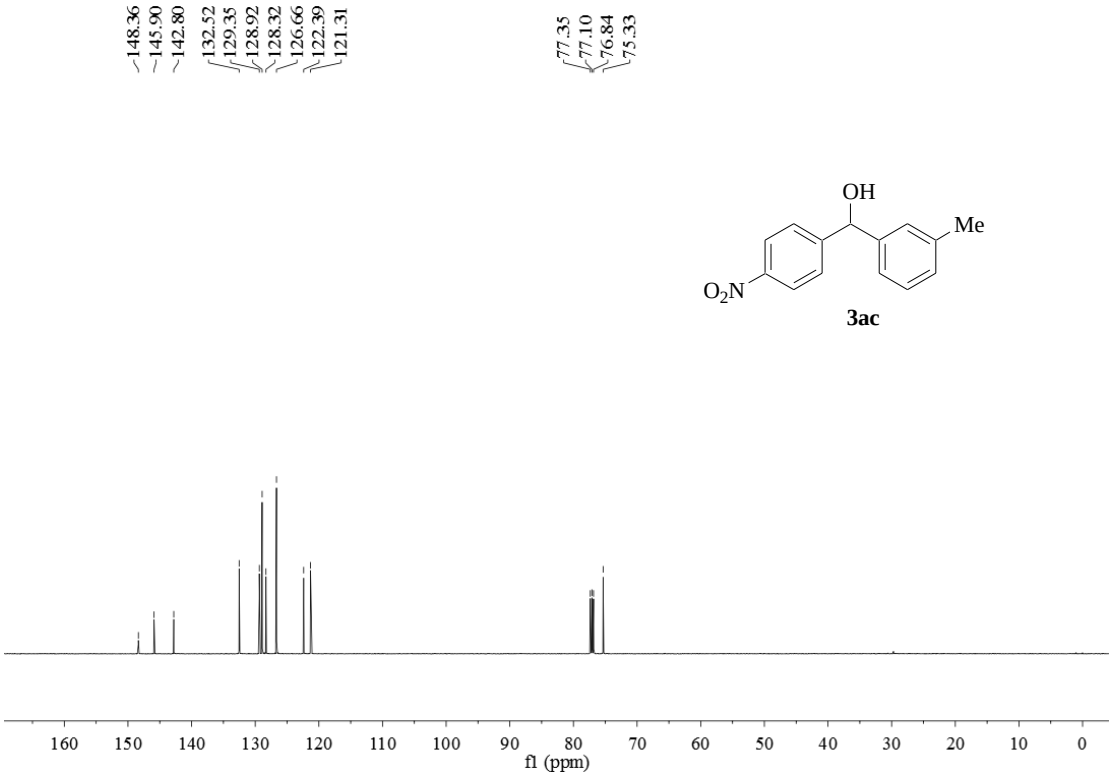
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75.33
OH
Me
O2N
3ac
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90
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50
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30
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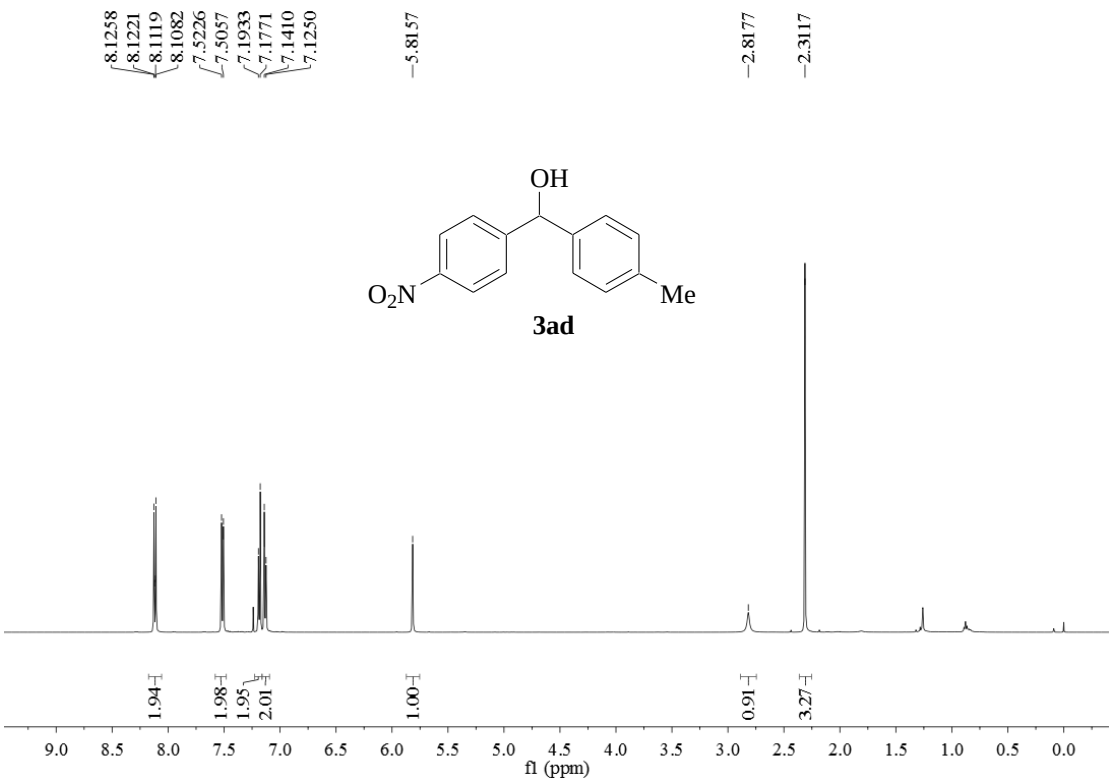
10
0
f1 (ppm)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2.3117
OH
O2N
Me
3ad
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1.98
1.95
2.01
1.00
0.91
3.27
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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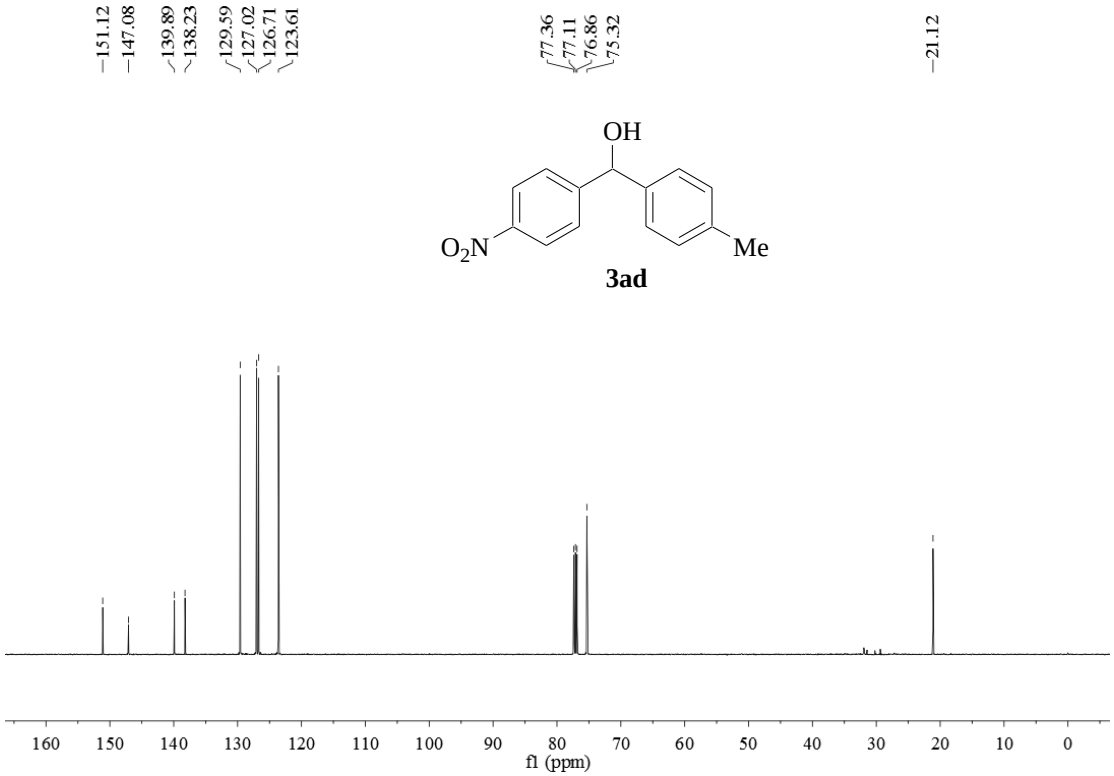
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123.61
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77.11
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75.32
21.12
OH
O2N
Me
3ad
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130
120
110
100
90
80
70
60
50
40
30
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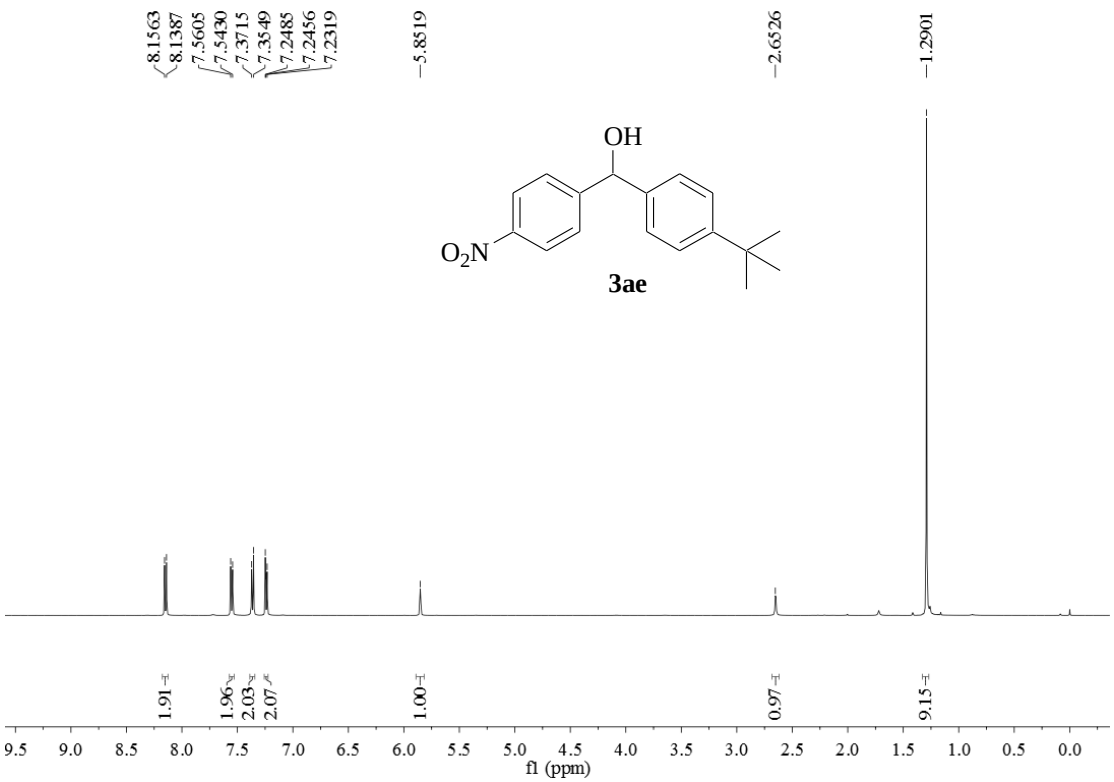
10
0
f1 (ppm)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7.2485
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7.2319
5.8519
2.6526
1.2901
OH
O2N
3ae
1.91
1.96
2.03
2.07
1.00
0.97
9.15
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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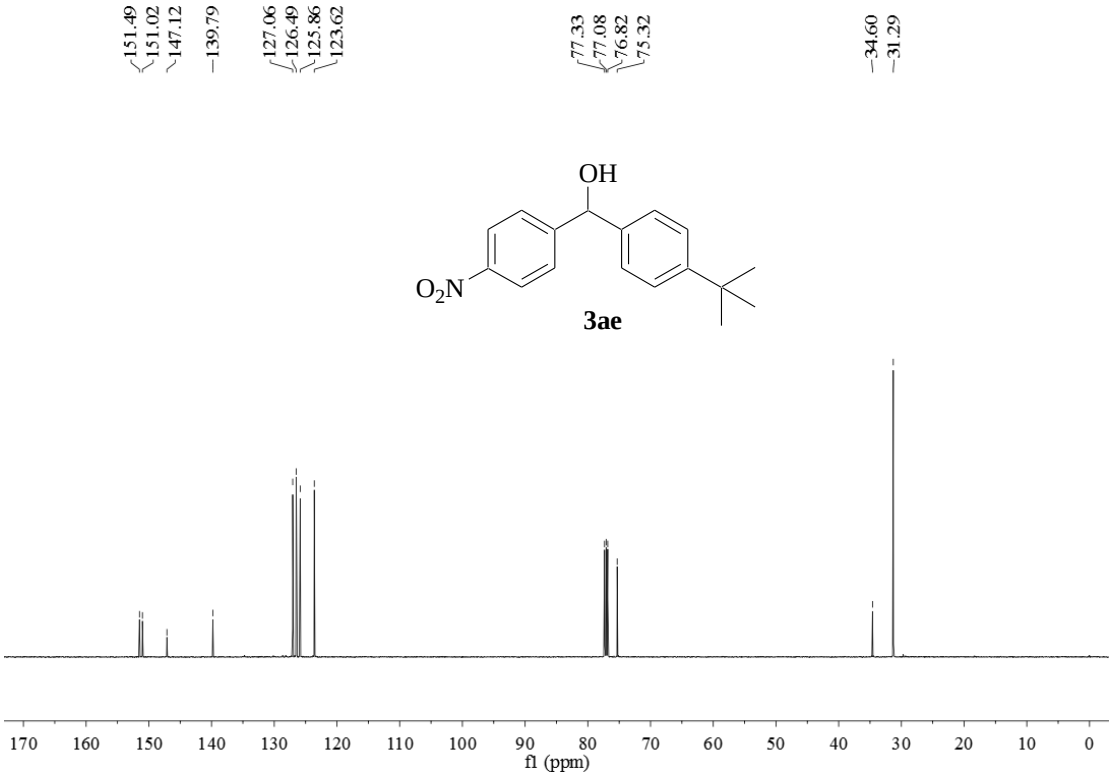
f1 (ppm)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126.49
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77.33
77.08
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34.60
31.29
OH
O2N
3ae
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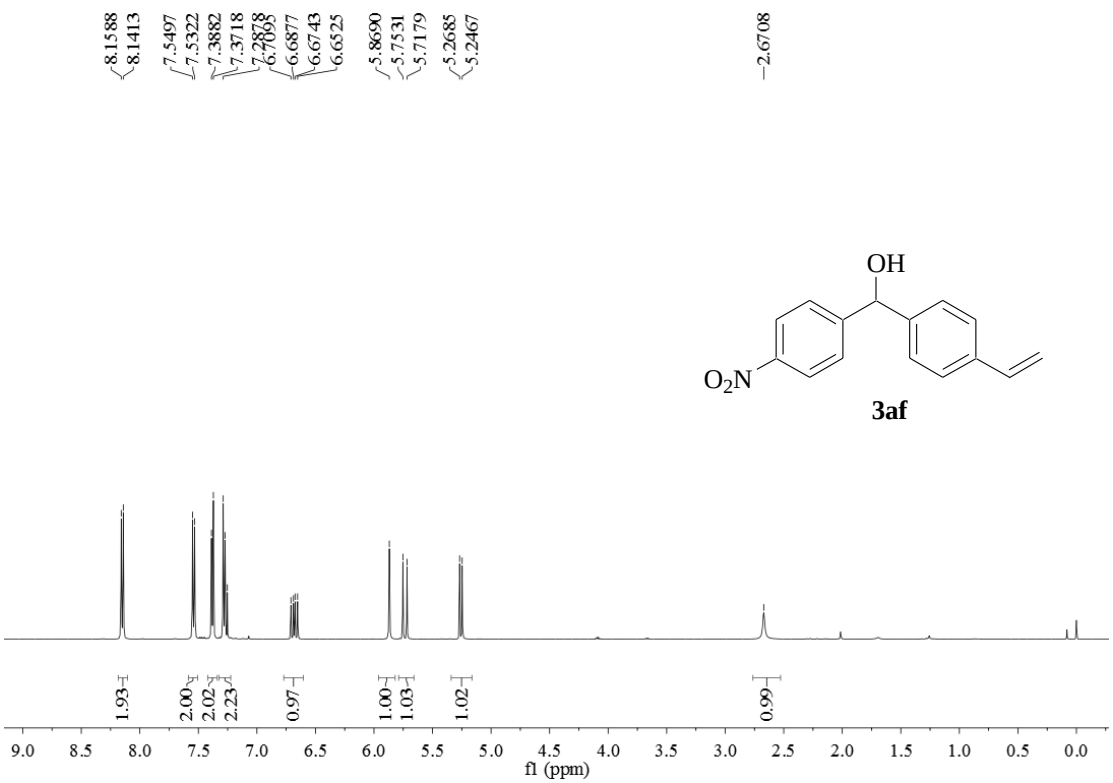
f1 (ppm)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5.7531
5.7179
5.2685
5.2467
2.6708
OH
O2N
3af
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2.00
2.02
2.23
0.97
1.00
1.03
1.02
0.99
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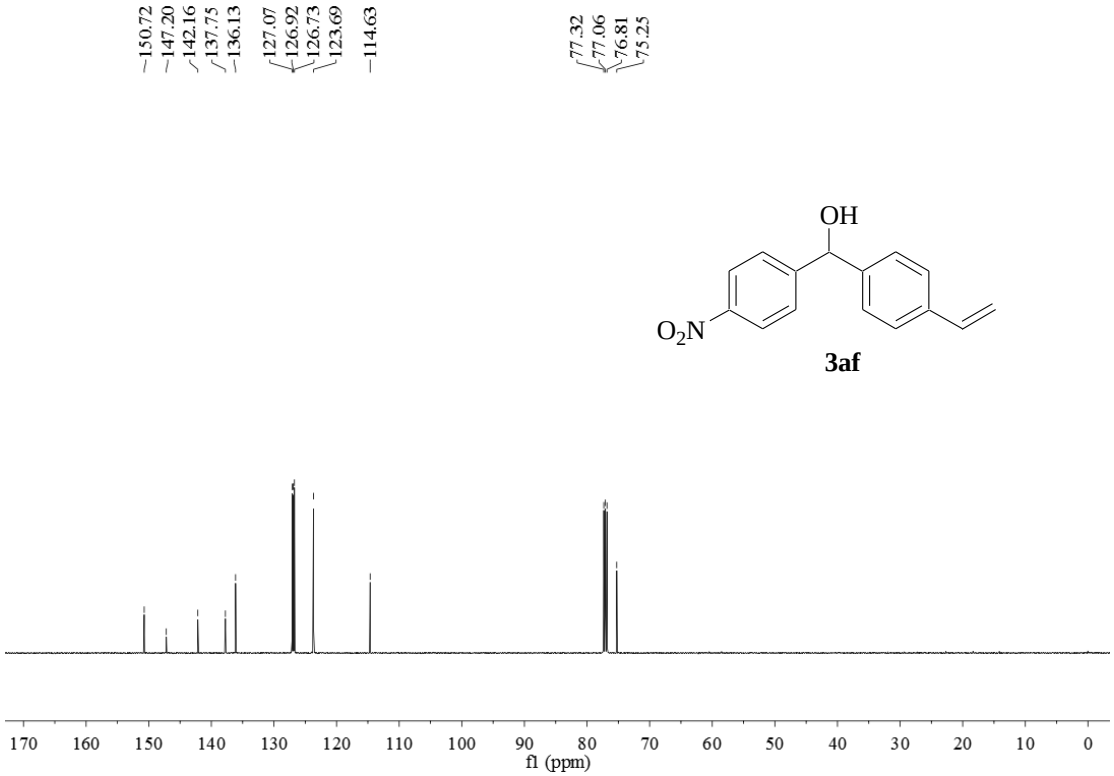
f1 (ppm)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75.25
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O2N
3af
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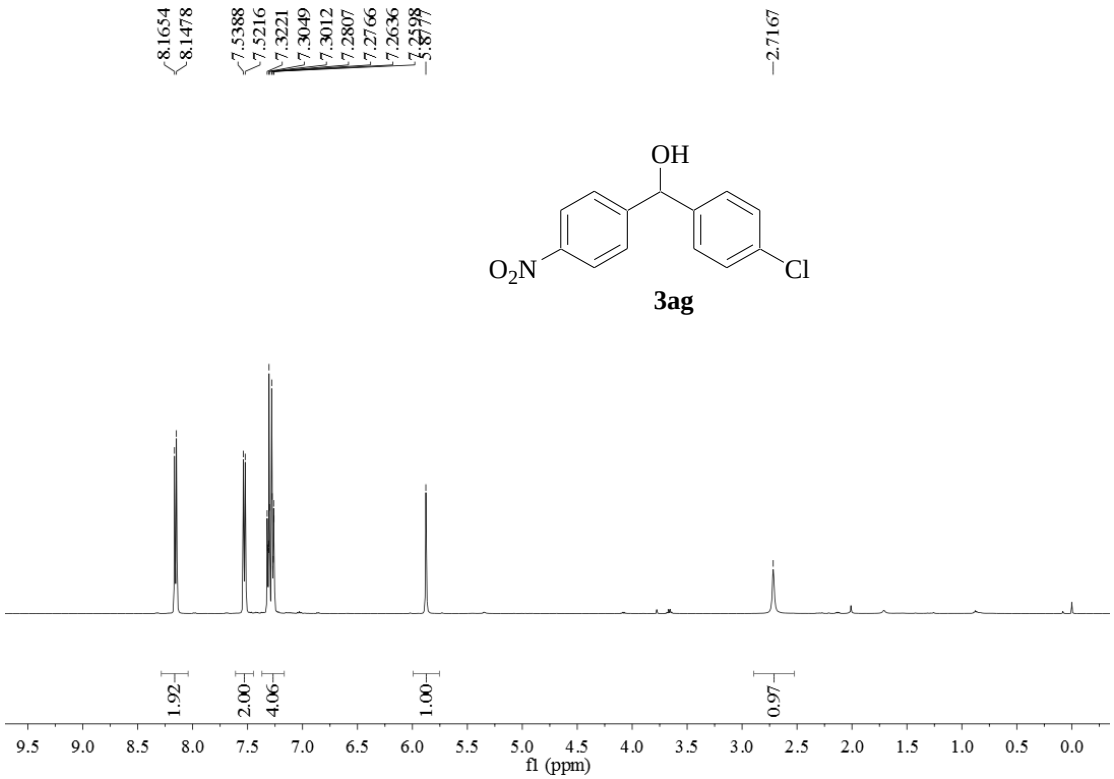
f1 (ppm)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5.8777
2.7167
OH
O2N
Cl
3ag
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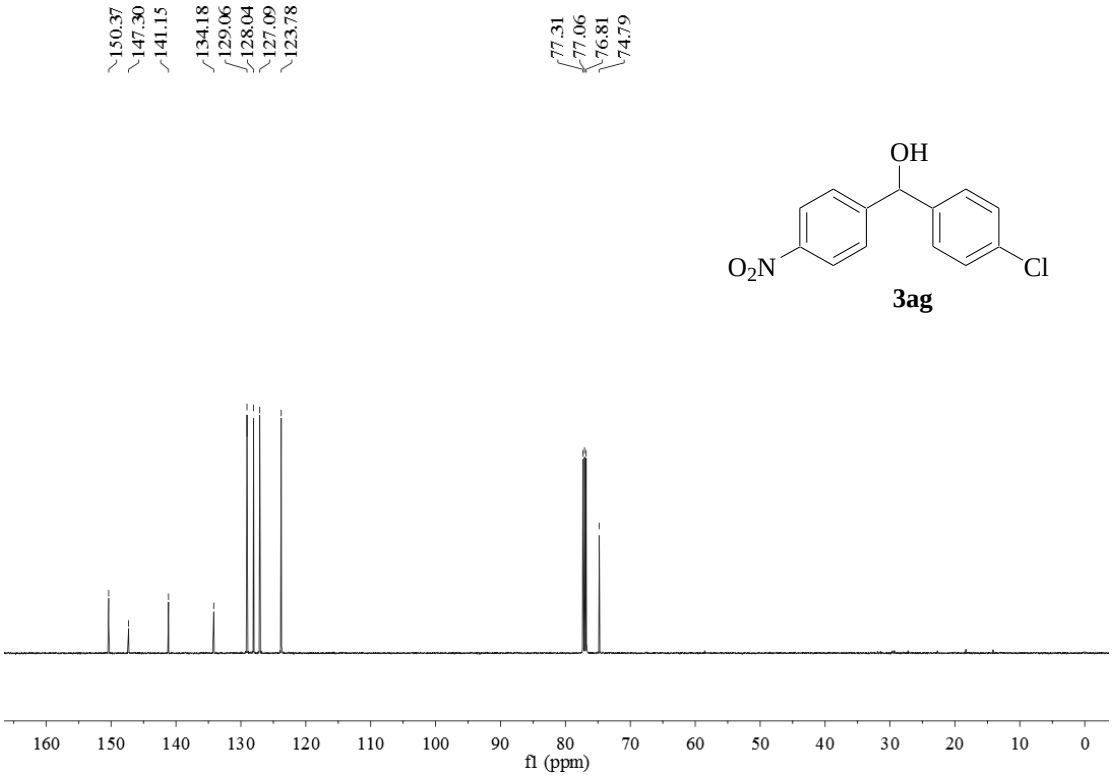
2.00
4.06
1.00
0.97
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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O2N
Cl
3ag
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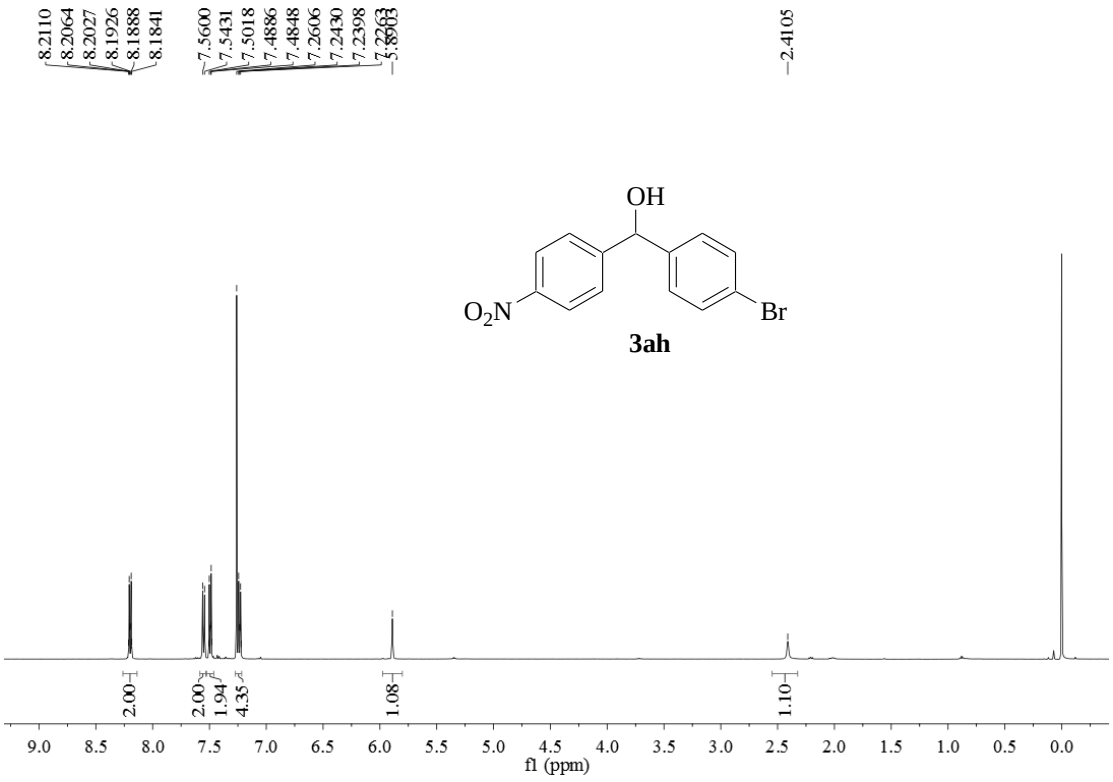
f1 (ppm)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7.4848
7.2606
7.2430
7.2398
2.4105
OH
O2N
Br
3ah
2.00
2.00
1.94
4.35
1.08
1.10
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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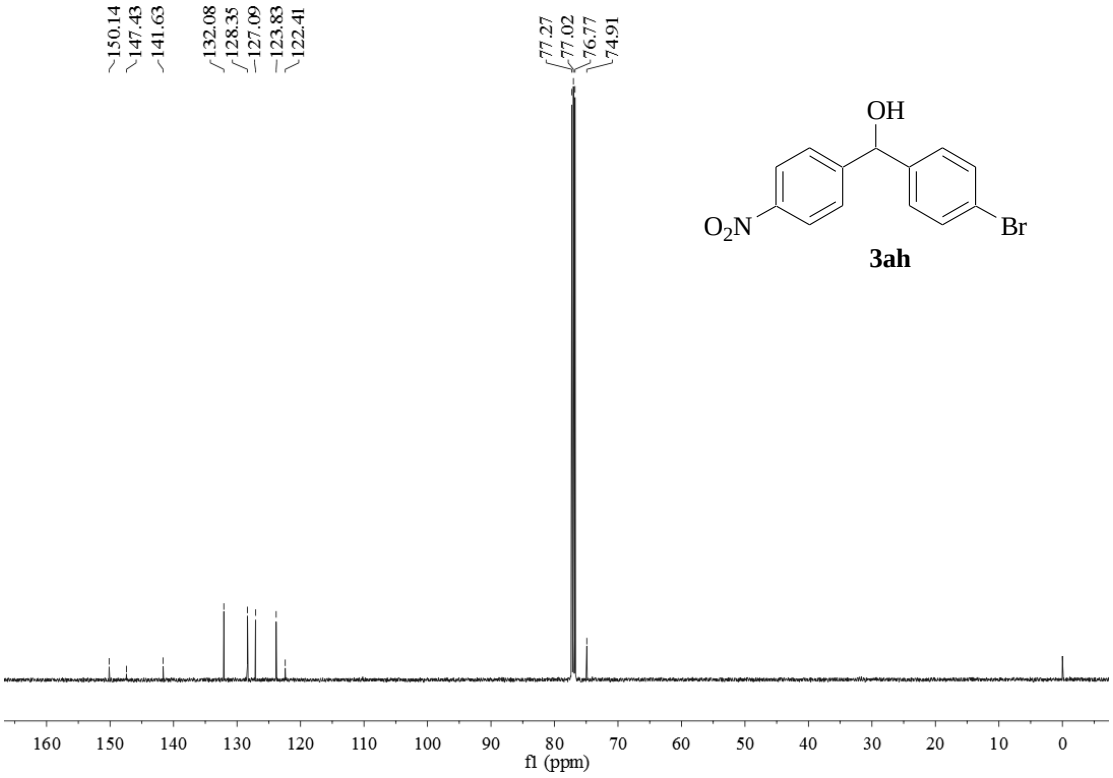
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O2N
Br
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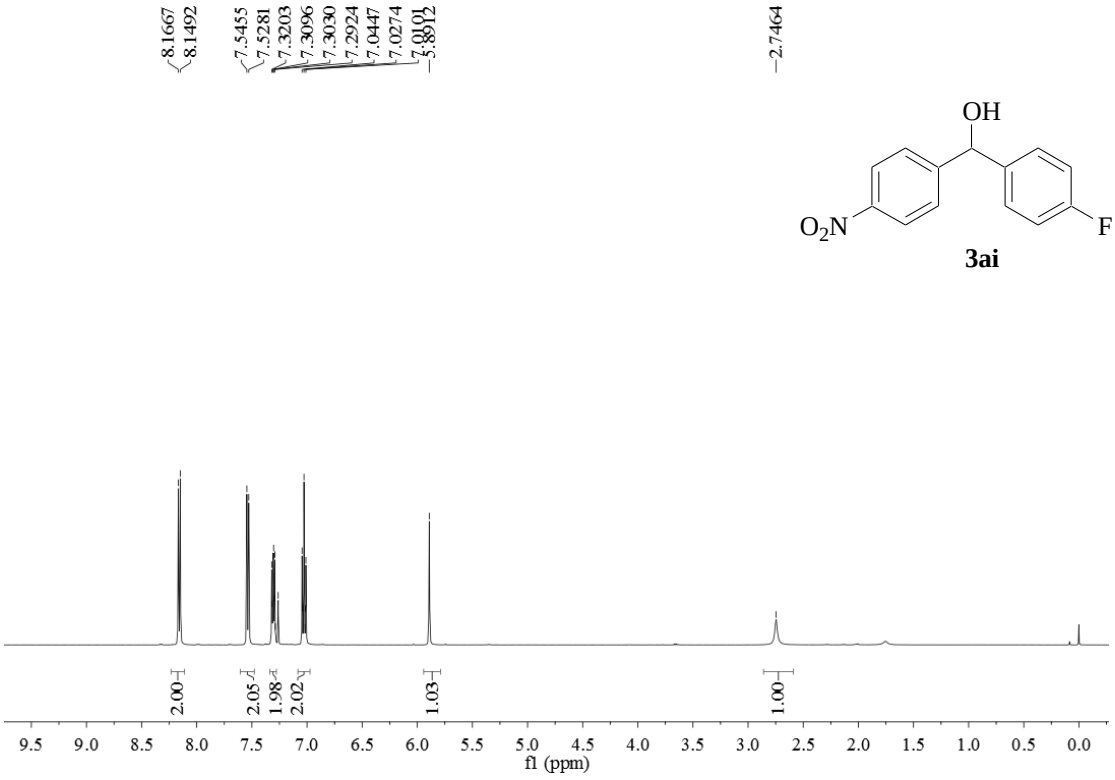
f1 (ppm)

3ah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7.0101
5.8912
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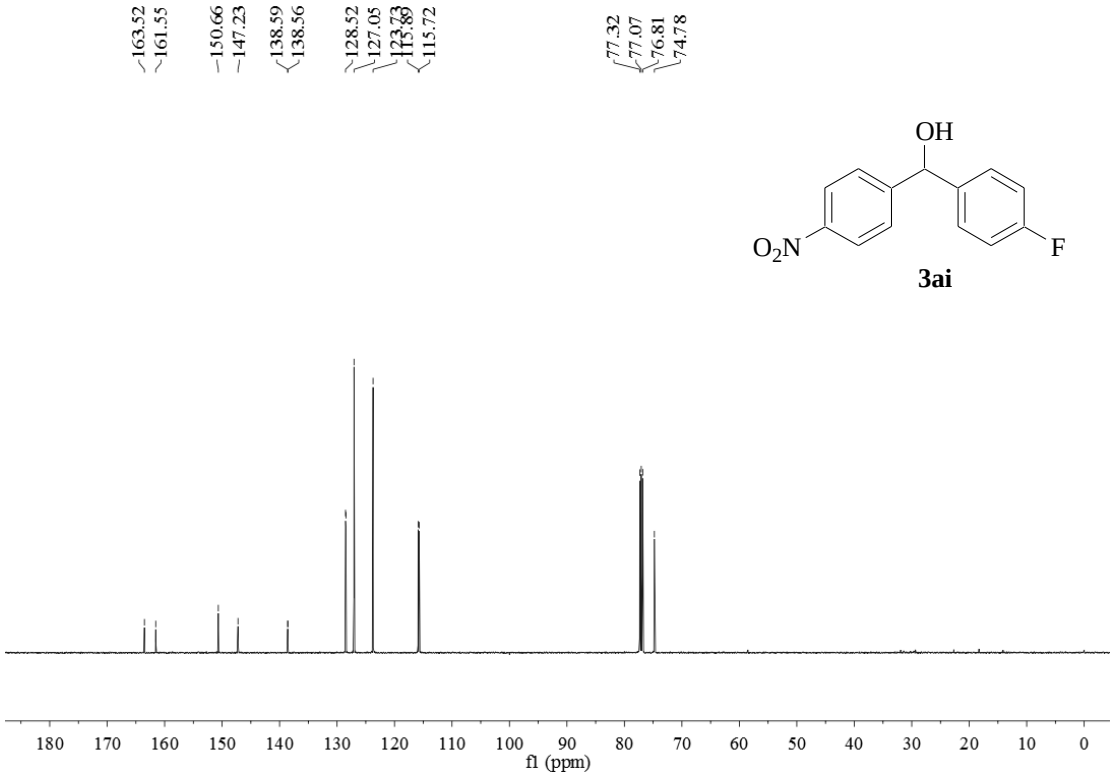
OH
O2N
F
2.00
2.05
1.98
2.02
1.03
1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3ai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138.56
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123.69
115.72
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77.07
76.81
74.78
OH
O2N
F
3ai
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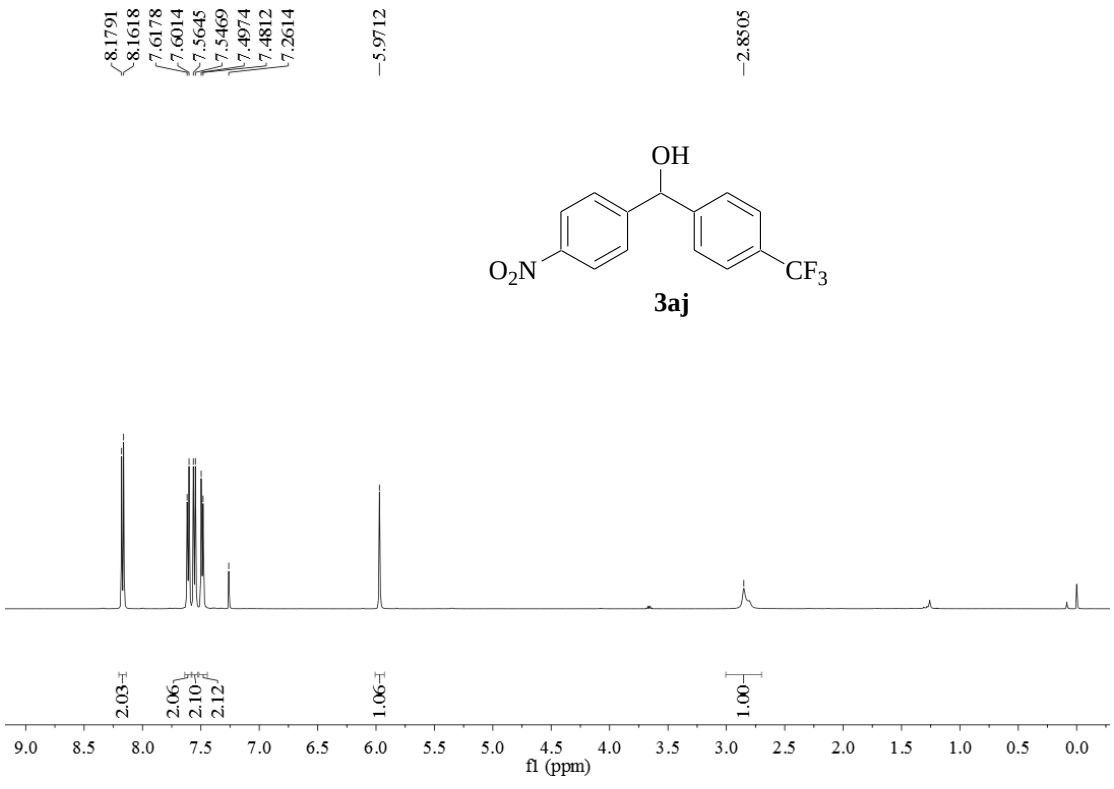
f1 (ppm)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CF3
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2.06
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2.12
1.06
1.00
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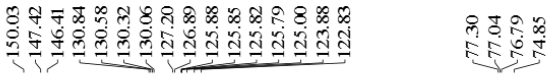
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122.83
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77.04
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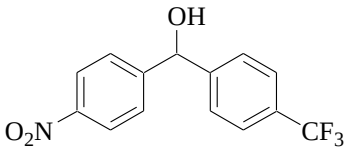
74.85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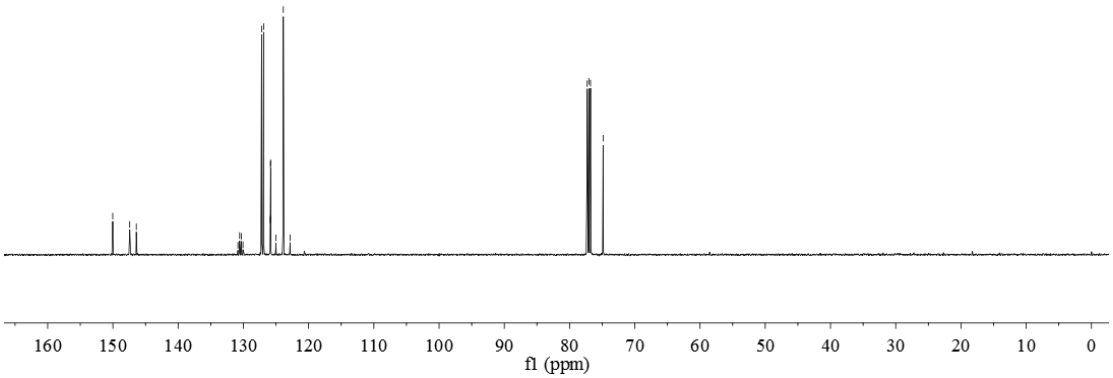
O2N
CF3

3aj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50
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20
10
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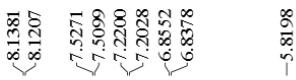
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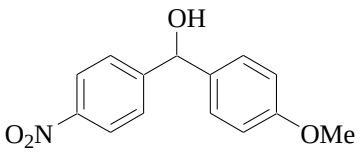
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OMe

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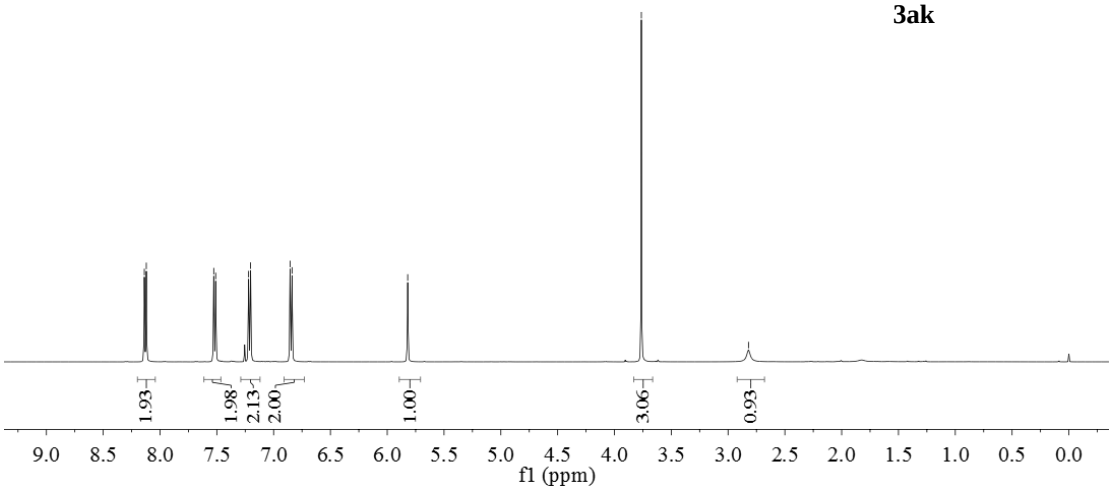
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6.5
6.0
5.5
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3.5
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2.0
1.5
1.0
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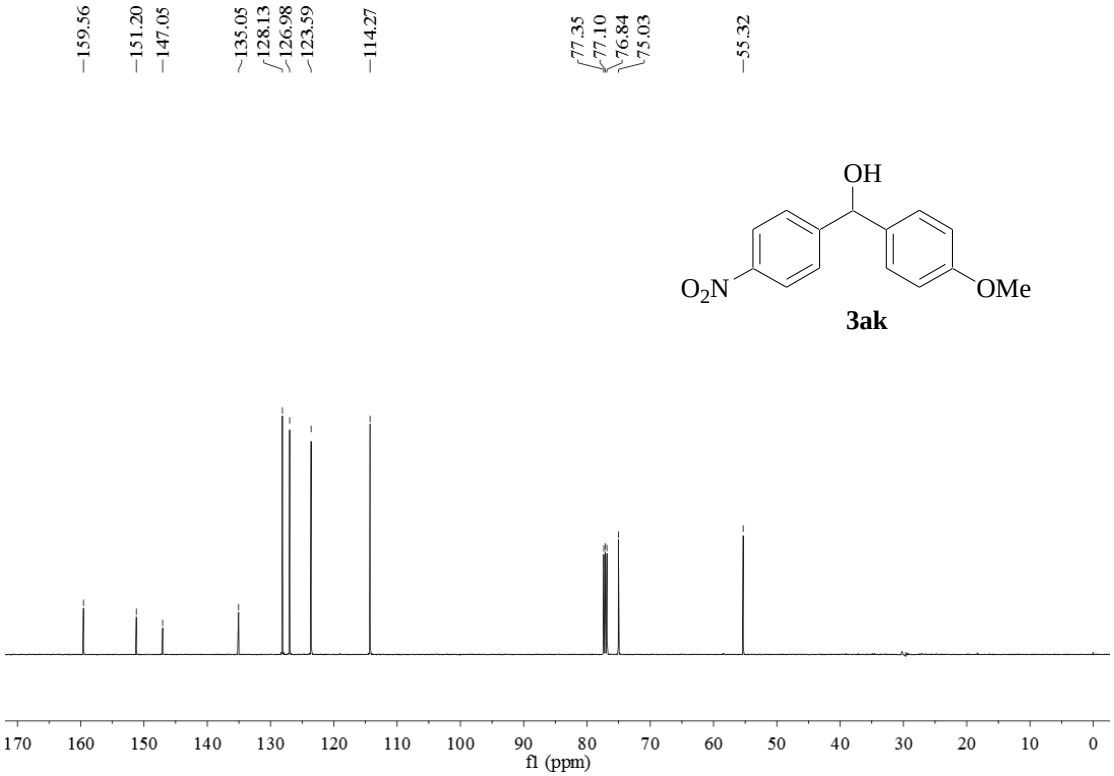
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114.27
77.35
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55.32
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OMe
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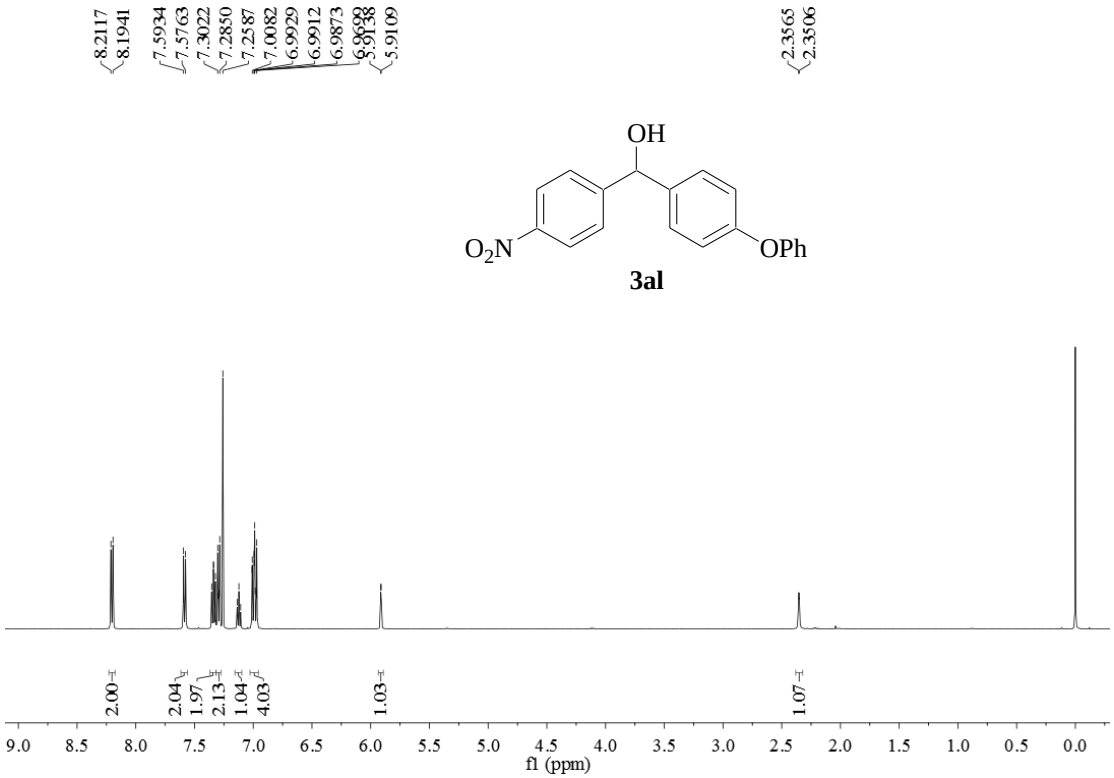
f1 (ppm)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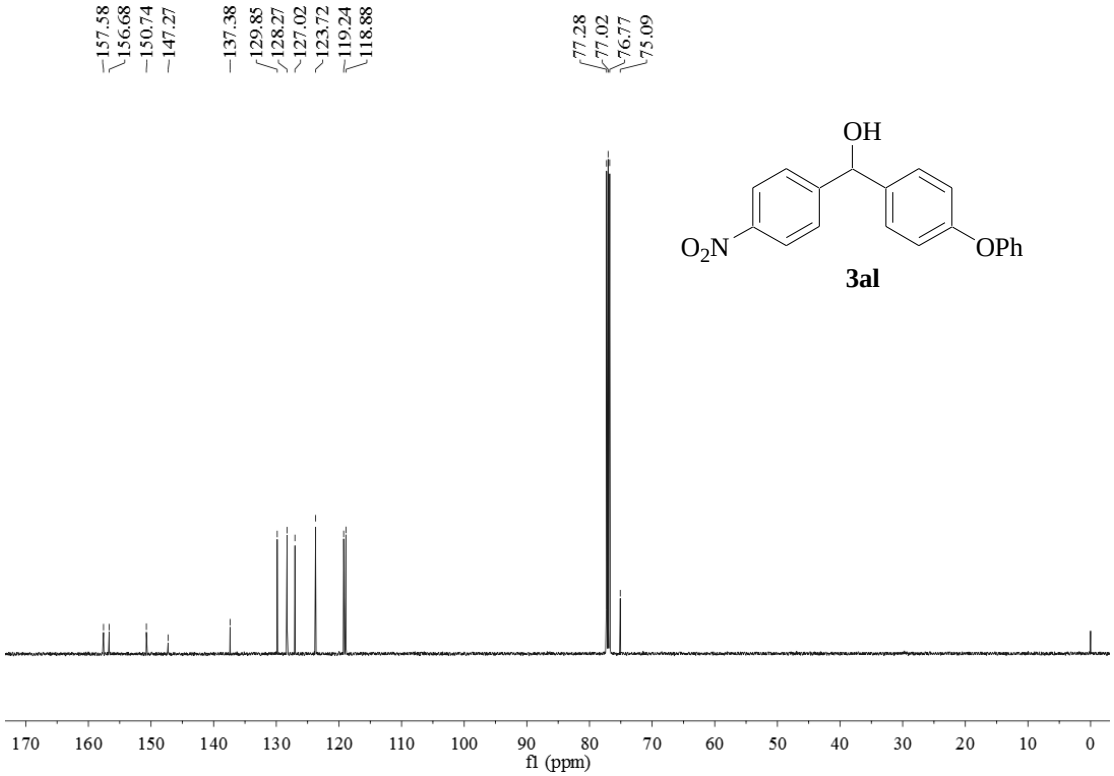
2.3506
OH
O2N
OPh
3al
2.00
2.04
1.97
2.13
1.04
4.03
1.03
1.07
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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75.09
OH
O2N
OPh
3al
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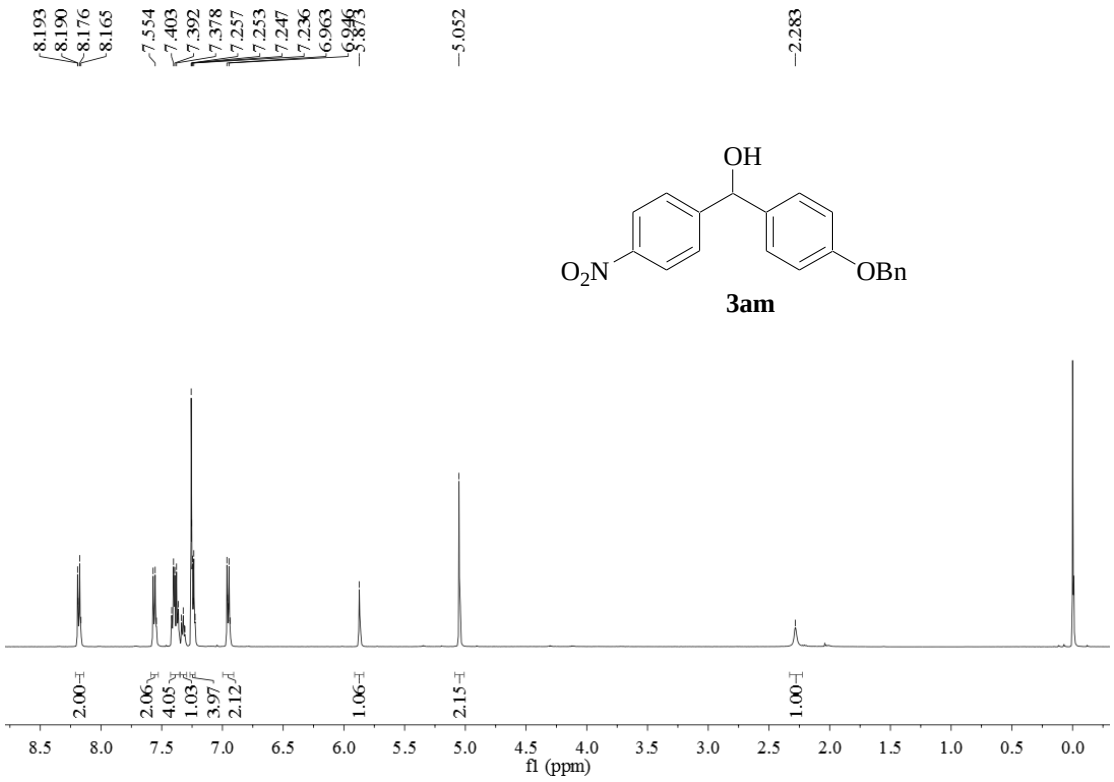
f1 (ppm)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7.247
7.236
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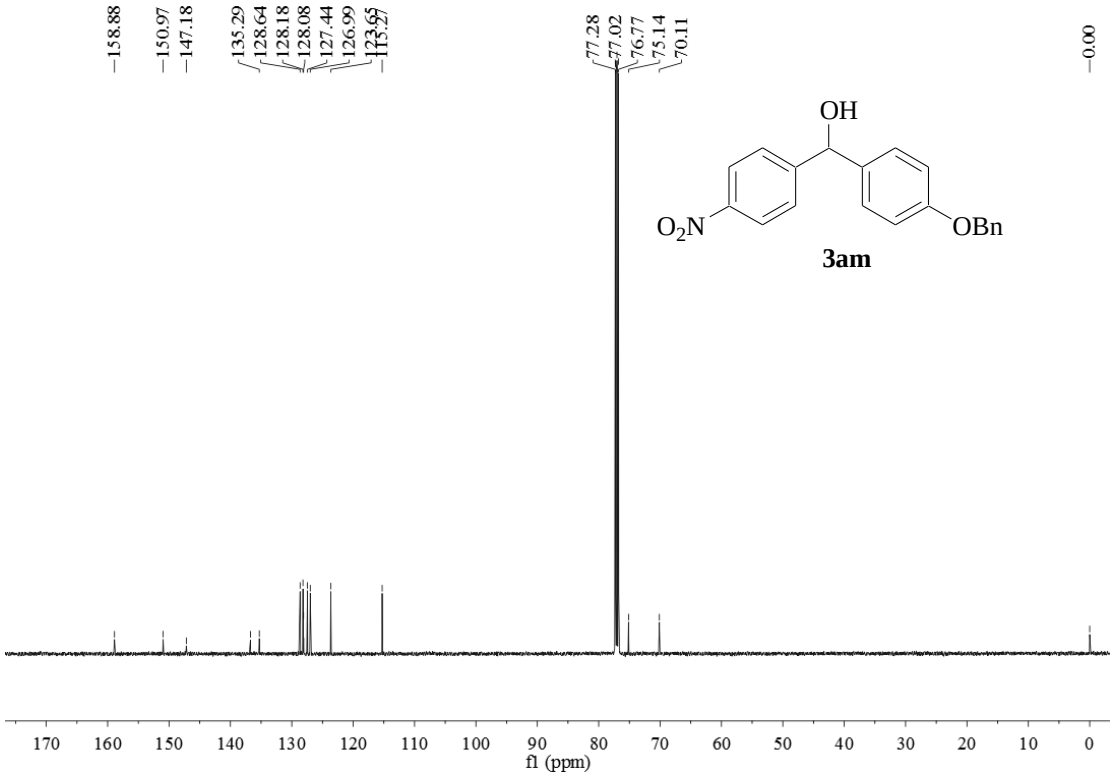
6.946
6.873
5.052
2.283
OH
O2N
OBn
3am
2.00
2.06
4.05
1.03
3.97
2.12
1.06
2.15
1.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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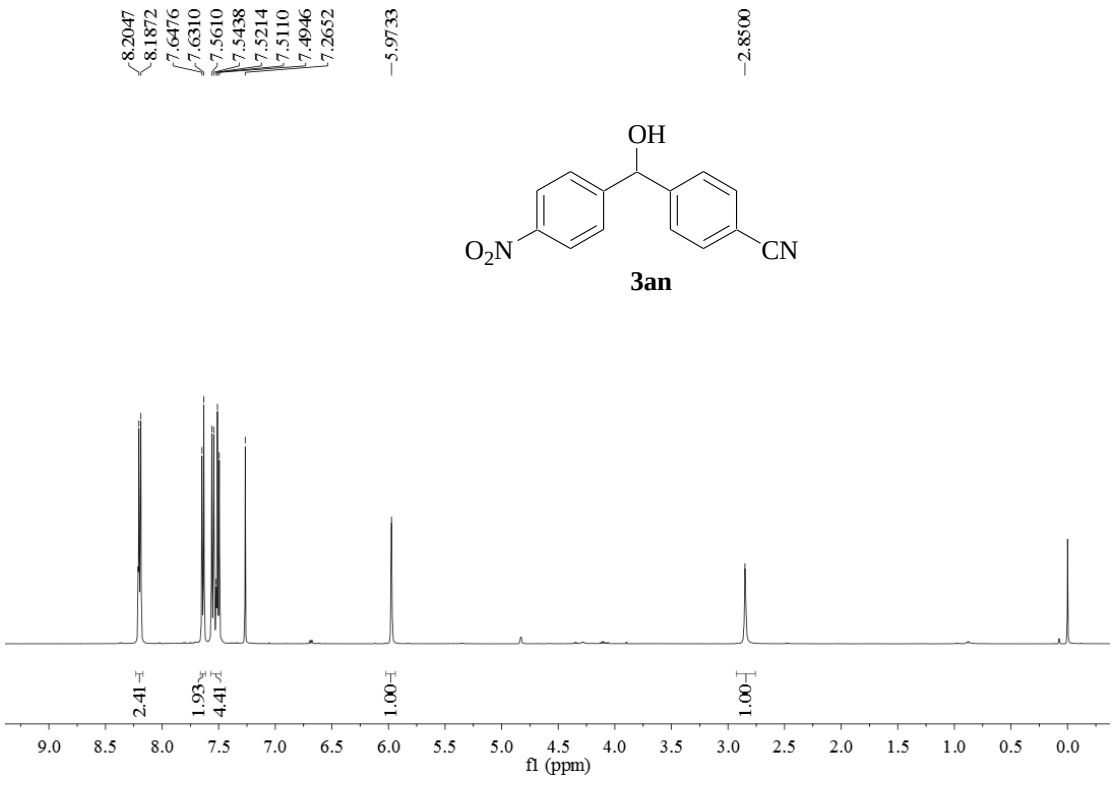
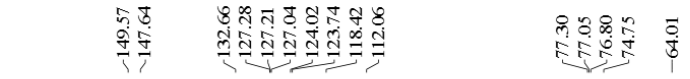
128.18
128.08
127.44
126.99
77.28
77.02
76.77
75.14
70.11
0.00
OH
O2N
OBn
3am
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.2047
8.1872
7.6476
7.6310
7.5610
7.5438
7.5214
7.5110
7.4946
7.2652
5.9733
2.8500
OH
O2N
CN
3an
2.41
1.93
4.41
1.00
1.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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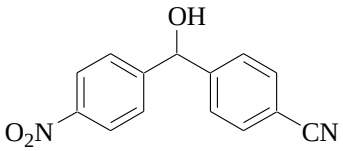
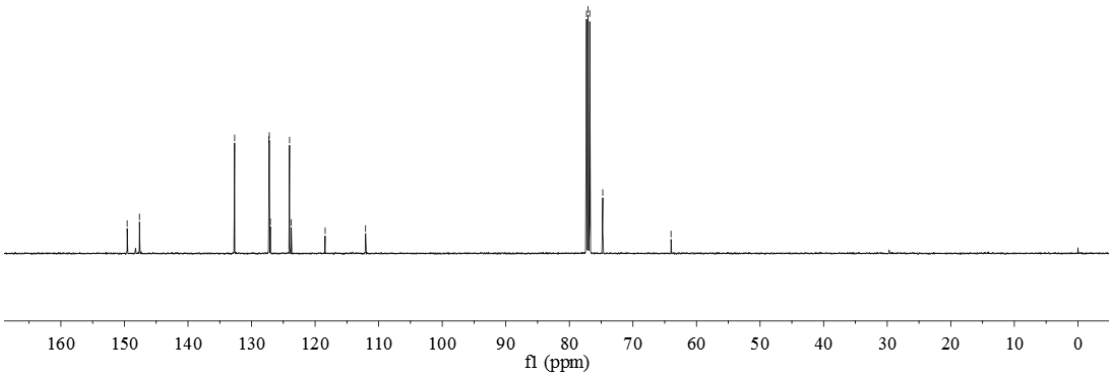
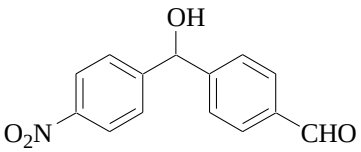
147.64
132.66
127.28
127.21
127.04
124.02
123.74
118.42
112.06
77.30
77.05
76.80
74.75
64.01


OH
O_2N
CN

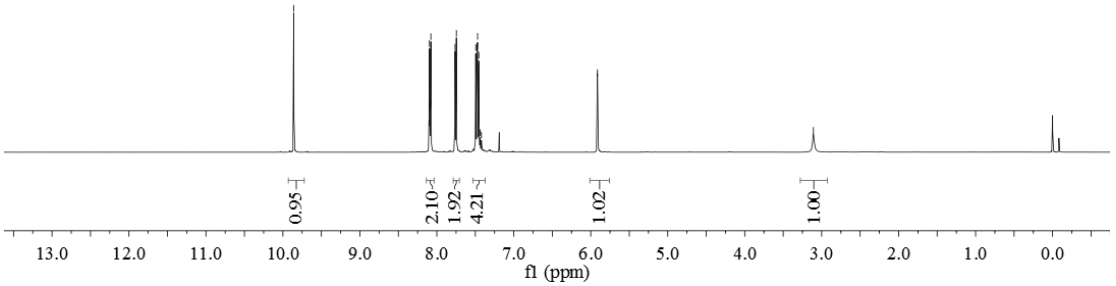
3an

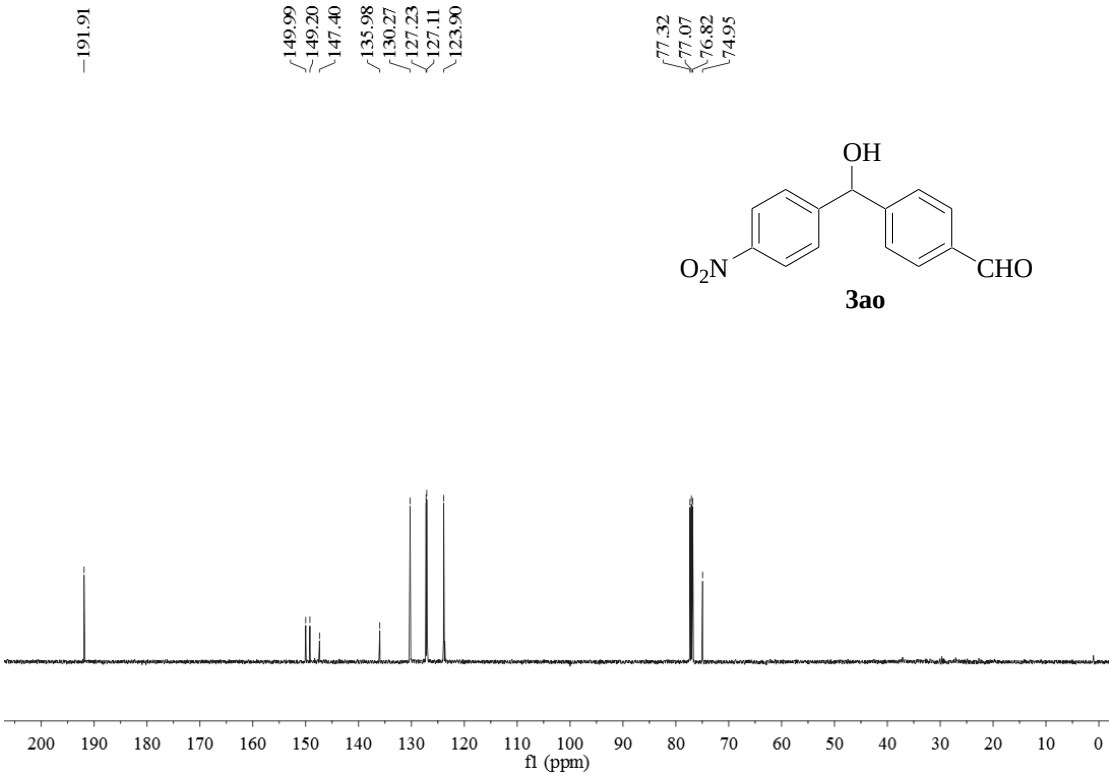

160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

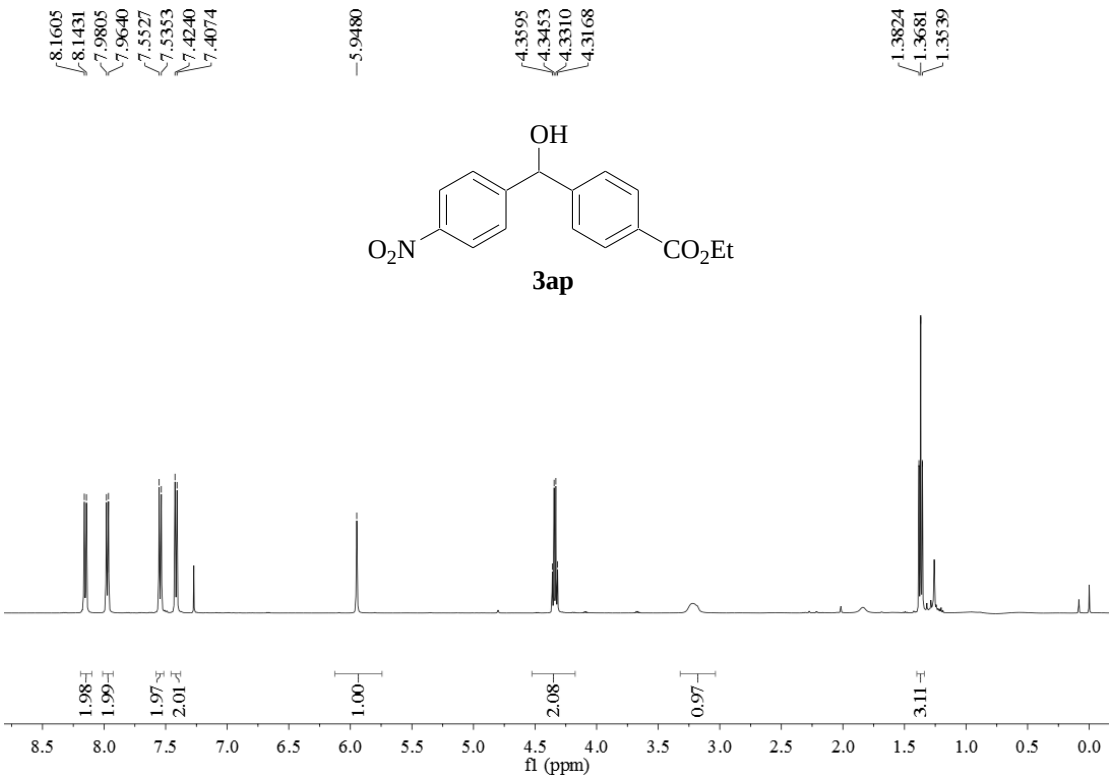

9.8593
8.1006
8.0955
8.0918
8.0816
8.0779
7.7629
7.7465
7.4946
7.4774
7.4709
7.4544
7.4385
5.9131
3.1073

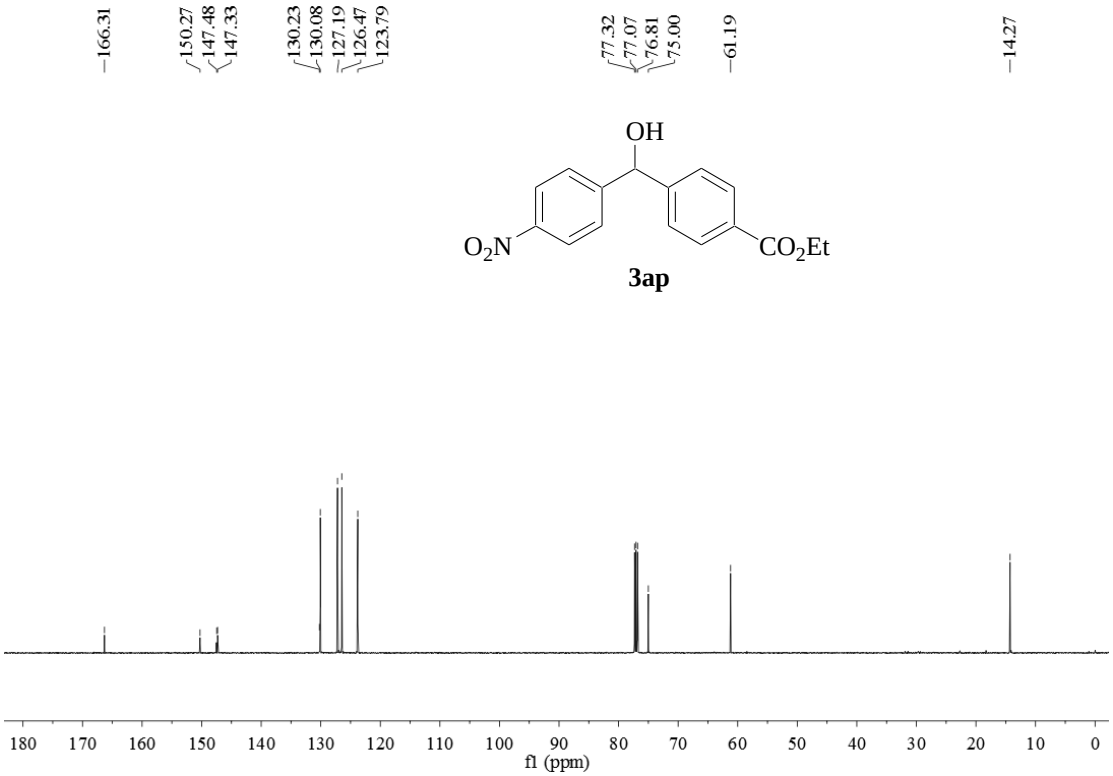

OH
O_2N
CHO

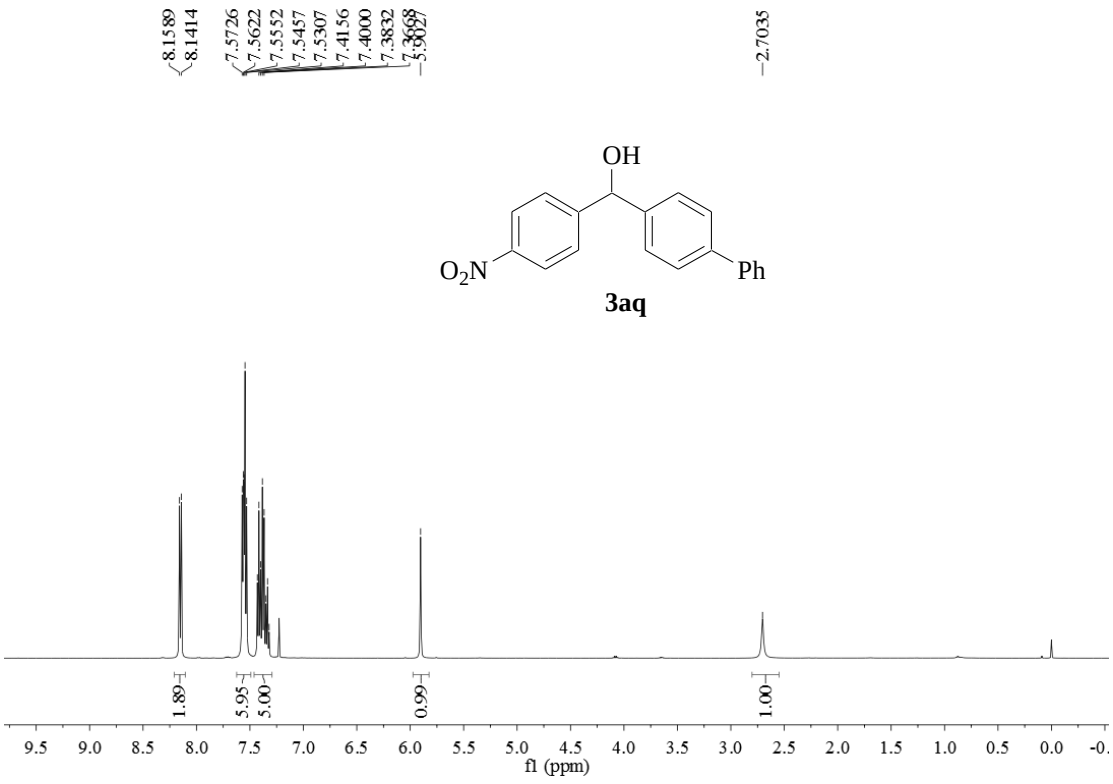
3ao

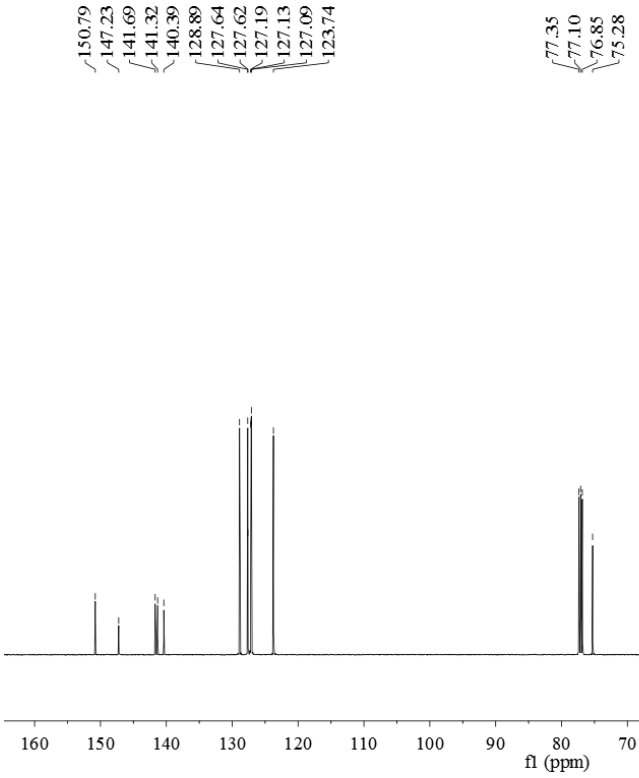

0.95
2.10
1.92
4.21
1.02
1.00
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

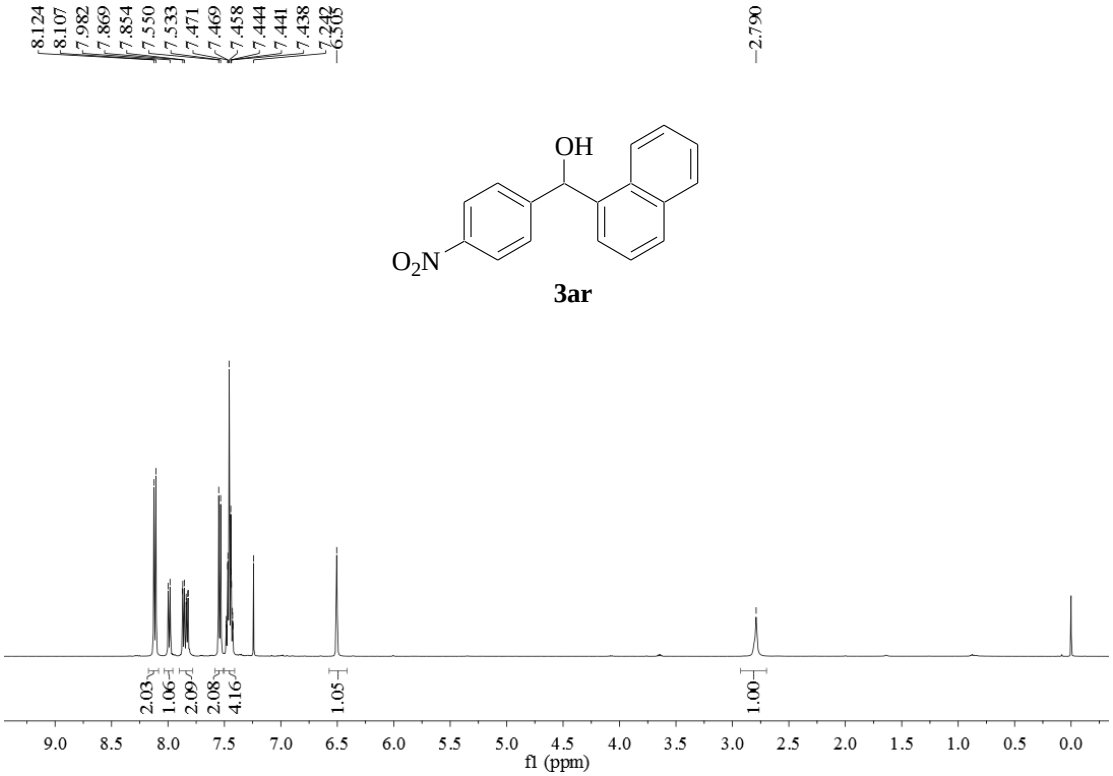

191.91
149.99
149.20
147.40
135.98
130.27
127.23
127.11
123.90
77.32
77.07
76.82
74.95
OH
O2N
CHO
3ao
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

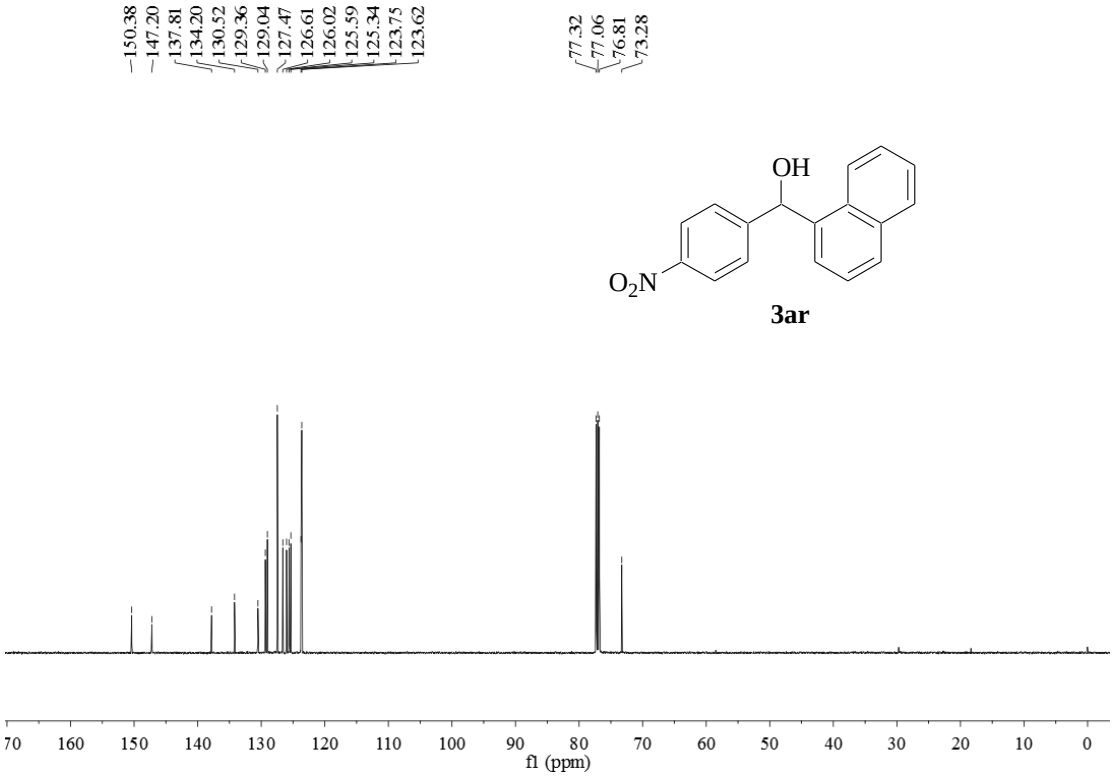

8.1605
8.1431
7.9805
7.9640
7.5527
7.5353
7.4240
7.4074
5.9480
4.3595
4.3453
4.3310
4.3168
1.3824
1.3681
1.3539
OH
O2N
CO2Et
3ap
1.98
1.99
1.97
2.01
1.00
2.08
0.97
3.11
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

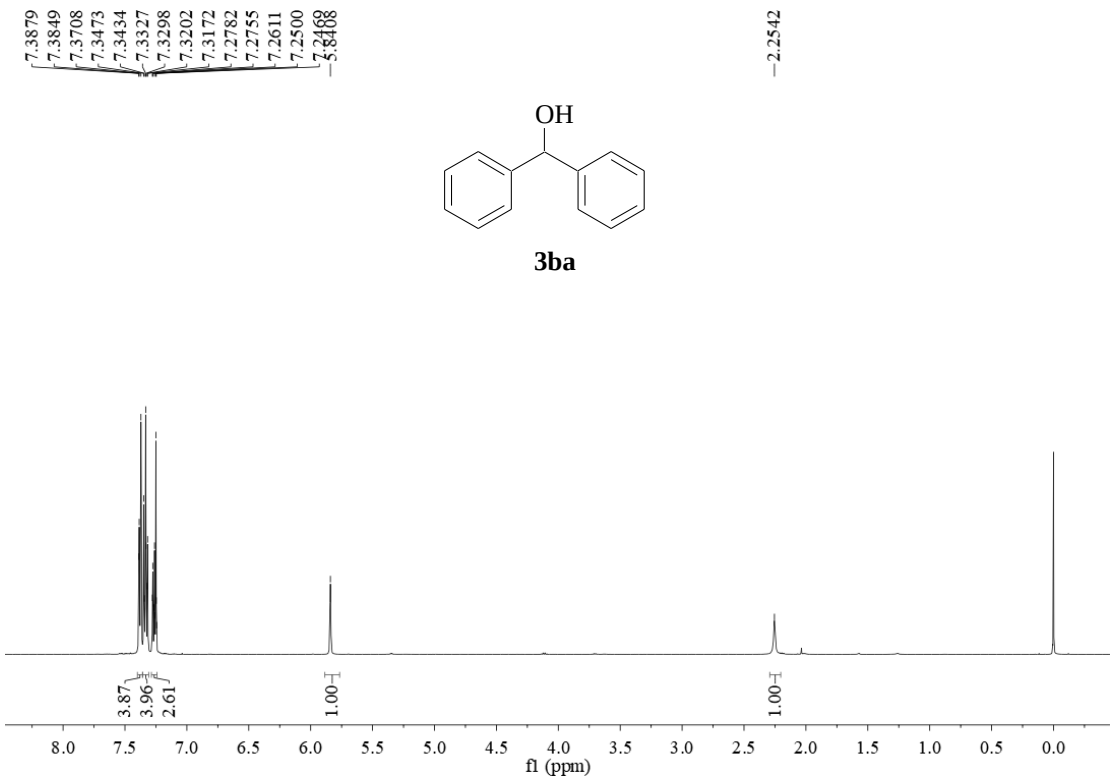

166.31
150.27
147.48
147.33
130.23
130.08
127.19
126.47
123.79
77.32
77.07
76.81
75.00
61.19
14.27
OH
O2N
CO2Et
3ap
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

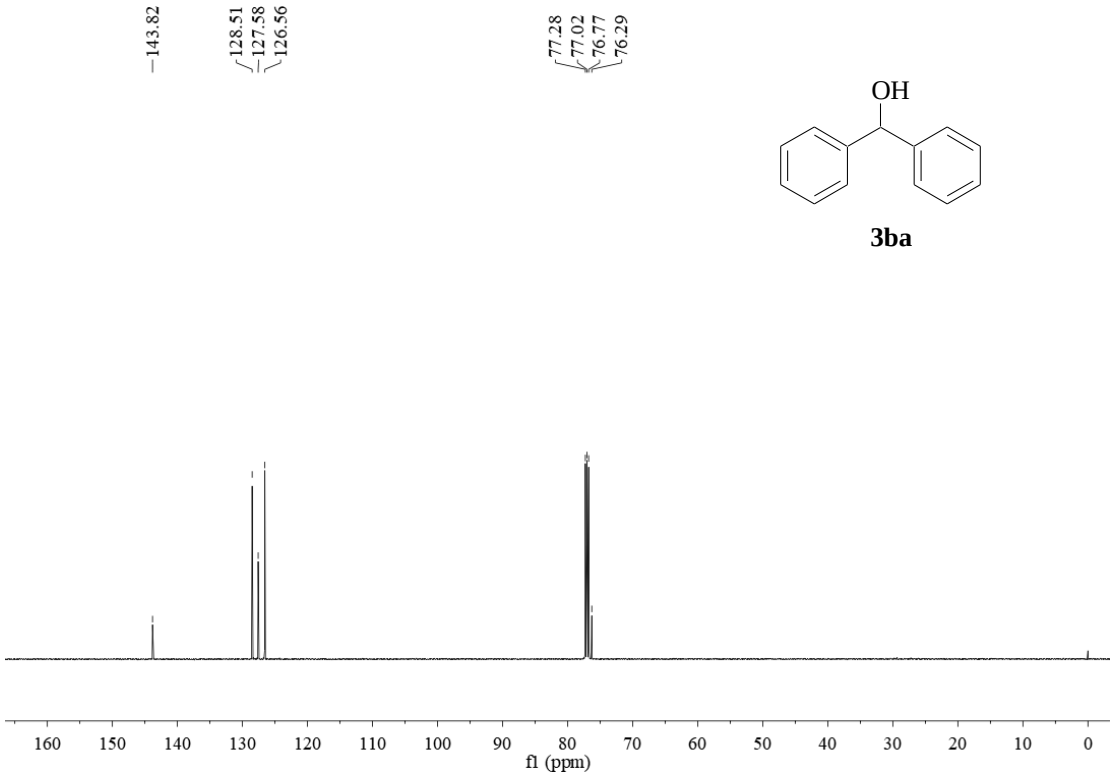

8.1589
8.1414
7.5726
7.5622
7.5552
7.5457
7.5307
7.4156
7.4000
7.3832
2.7035
OH
O2N
Ph
3aq
1.89
5.95
5.00
0.99
1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

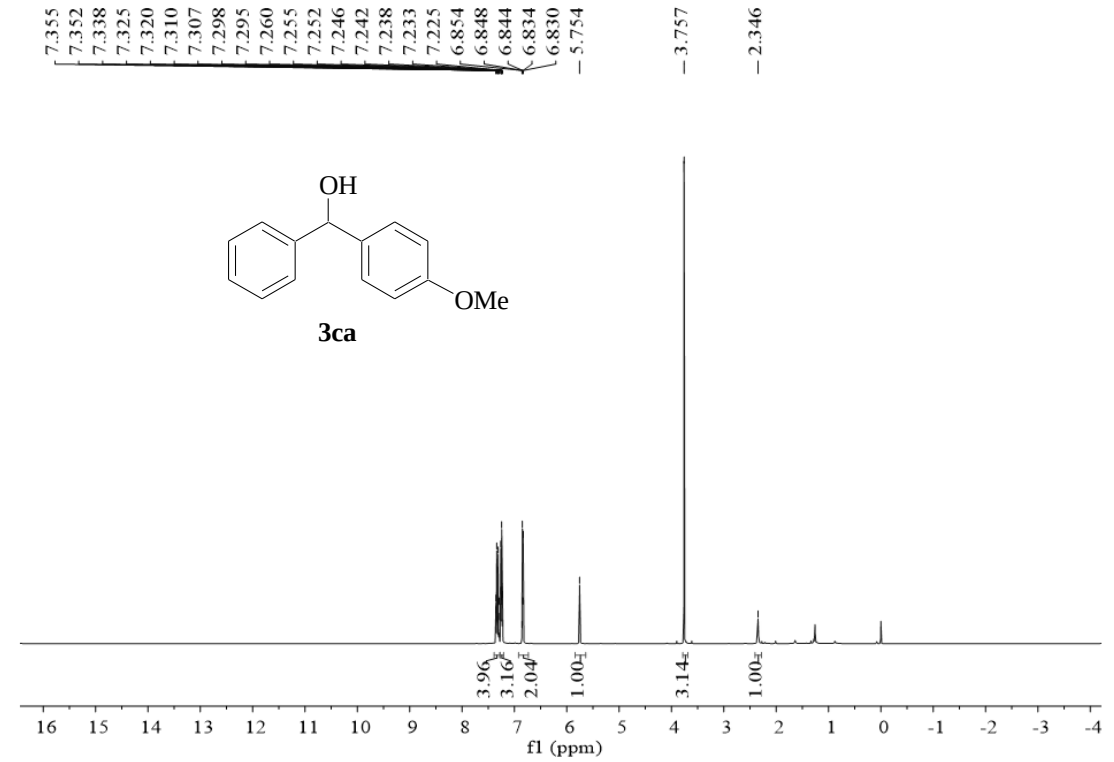

150.79
147.23
141.69
141.32
140.39
128.89
127.64
127.62
127.19
127.13
127.09
123.74
77.35
77.10
76.85
75.28
OH
O2N
Ph
3aq
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

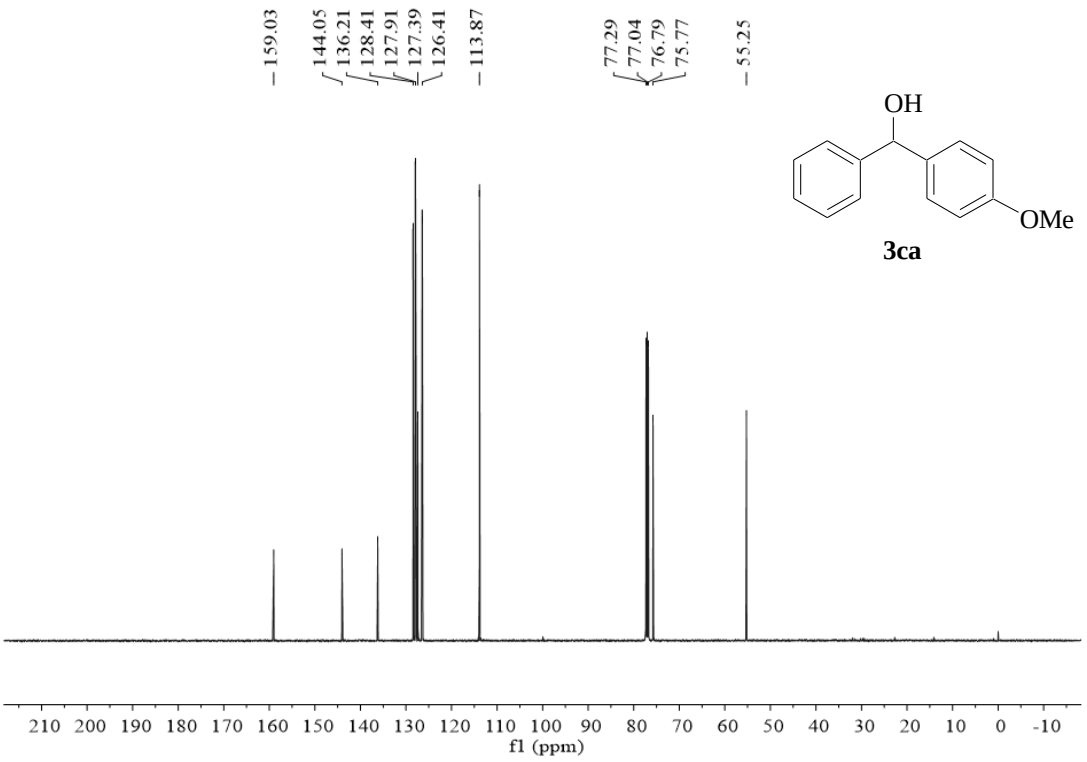

8.124
8.107
7.982
7.869
7.854
7.550
7.533
7.471
7.469
7.458
7.444
7.441
7.438
7.242
6.505
2.790
OH
O2N
3ar
2.03
1.06
2.09
2.08
4.16
1.05
1.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

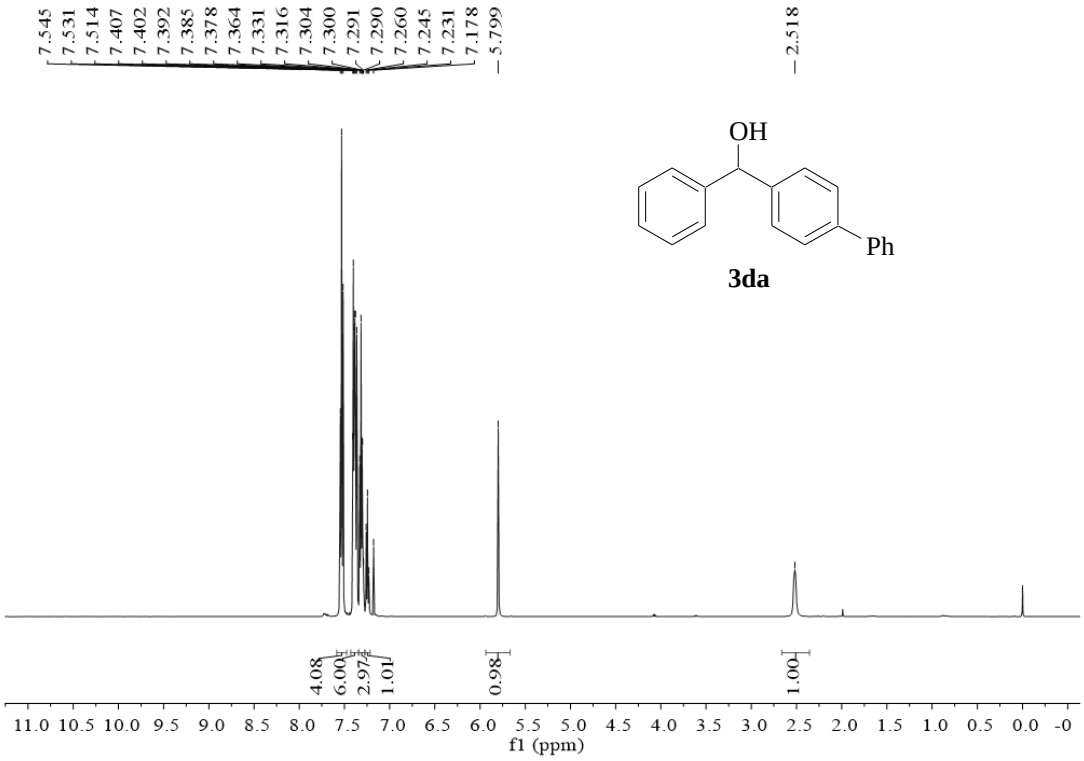

150.38
147.20
137.81
134.20
130.52
129.36
129.04
127.47
126.61
126.02
125.59
125.34
123.75
123.62
77.32
77.06
76.81
73.28
OH
O2N
3ar
70 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

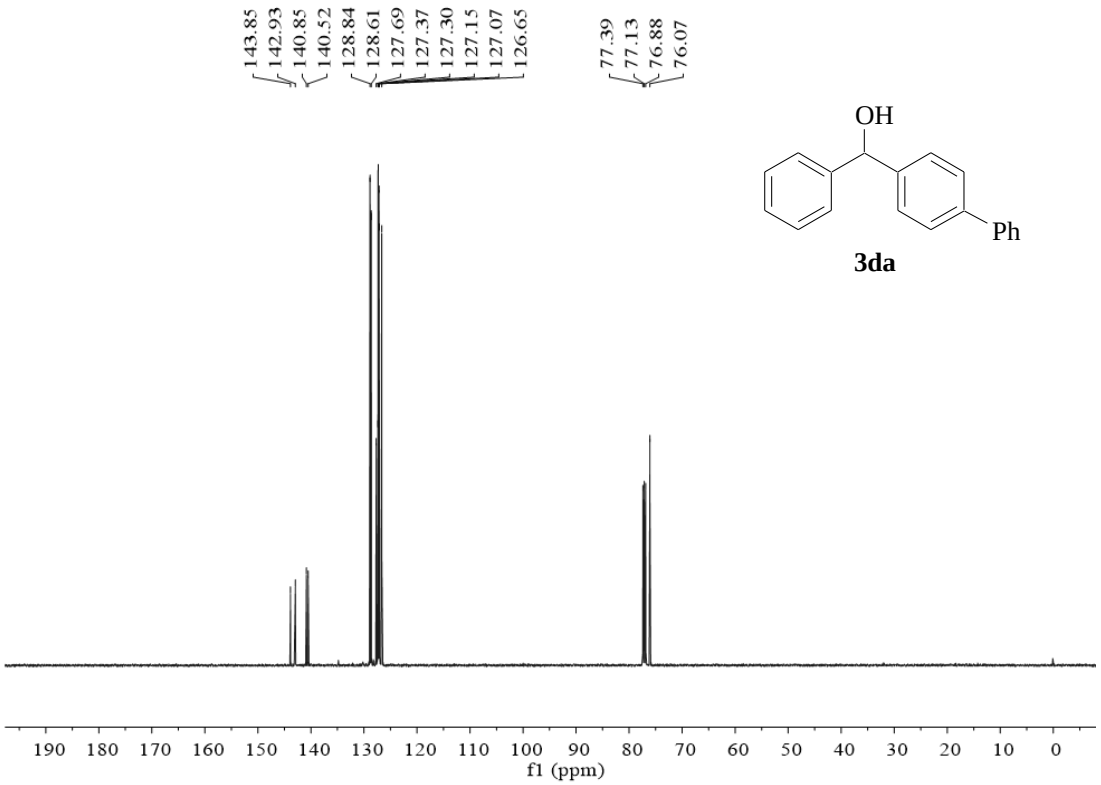

7.3879
7.3849
7.3708
7.3473
7.3434
7.3327
7.3298
7.3202
7.3172
7.2782
7.2755
7.2611
7.2500
7.2469
5.8408
2.2542
OH
3ba
3.87
3.96
2.61
1.00
1.00
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


143.82
128.51
127.58
126.56
77.28
77.02
76.77
76.29
OH
3ba
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

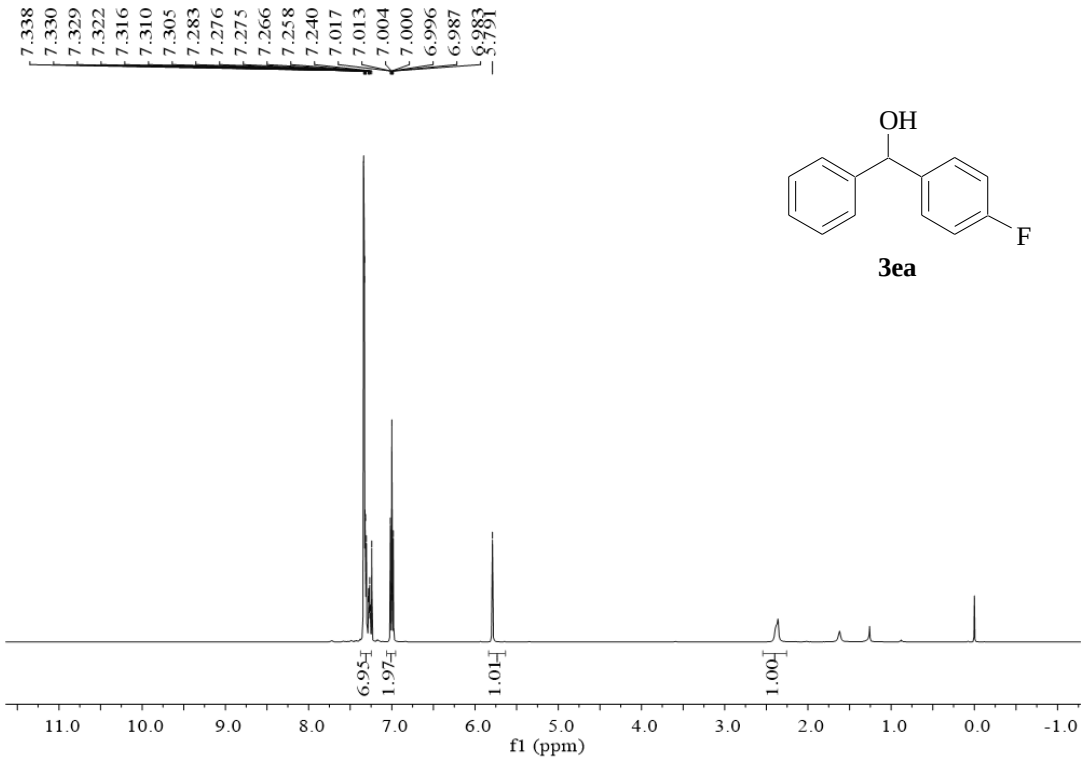

7.355
7.352
7.338
7.325
7.320
7.310
7.307
7.298
7.295
7.260
7.255
7.252
7.246
7.242
7.238
7.233
7.225
6.854
6.848
6.844
6.834
6.830
5.754
3.757
2.346
OH
OMe
3ca
3.96
3.16
2.04
1.00
3.14
1.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)


159.03
144.05
136.21
128.41
127.91
127.39
126.41
113.87
77.29
77.04
76.79
75.77
55.25
OH
OMe
3ca
f1 (ppm)

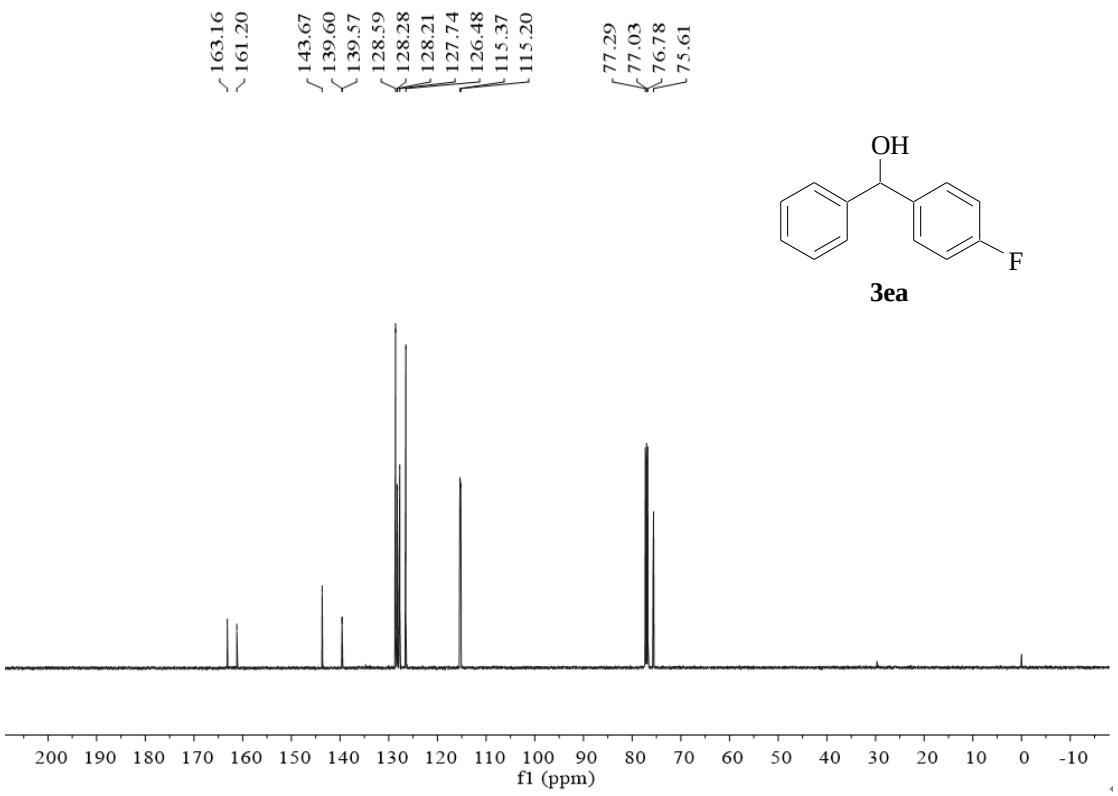

7.545
7.531
7.514
7.407
7.402
7.392
7.385
7.378
7.364
7.331
7.316
7.304
7.300
7.291
7.290
7.260
7.245
7.231
7.178
5.799
2.518
OH
Ph
3da
4.08
6.00
2.97
1.01
0.98
1.00
f1 (ppm)


143.85
142.93
140.85
140.52
128.84
128.61
127.69
127.37
127.30
127.15
127.07
126.65
77.39
77.13
76.88
76.07
OH
Ph
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

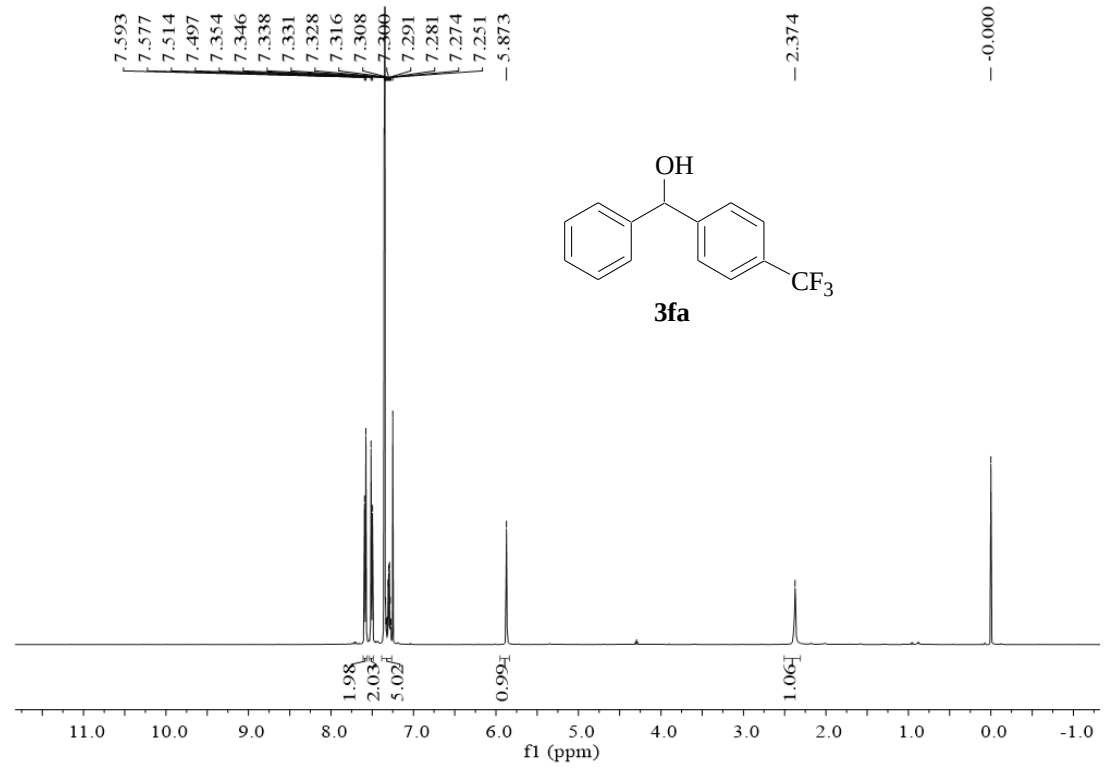
3da


7.338
7.330
7.329
7.322
7.316
7.310
7.305
7.283
7.276
7.275
7.266
7.258
7.240
7.017
7.013
7.004
7.000
6.996
6.987
6.983
5.791
OH
F
6.95
1.97
1.01
1.00
11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1.0
f1 (ppm)

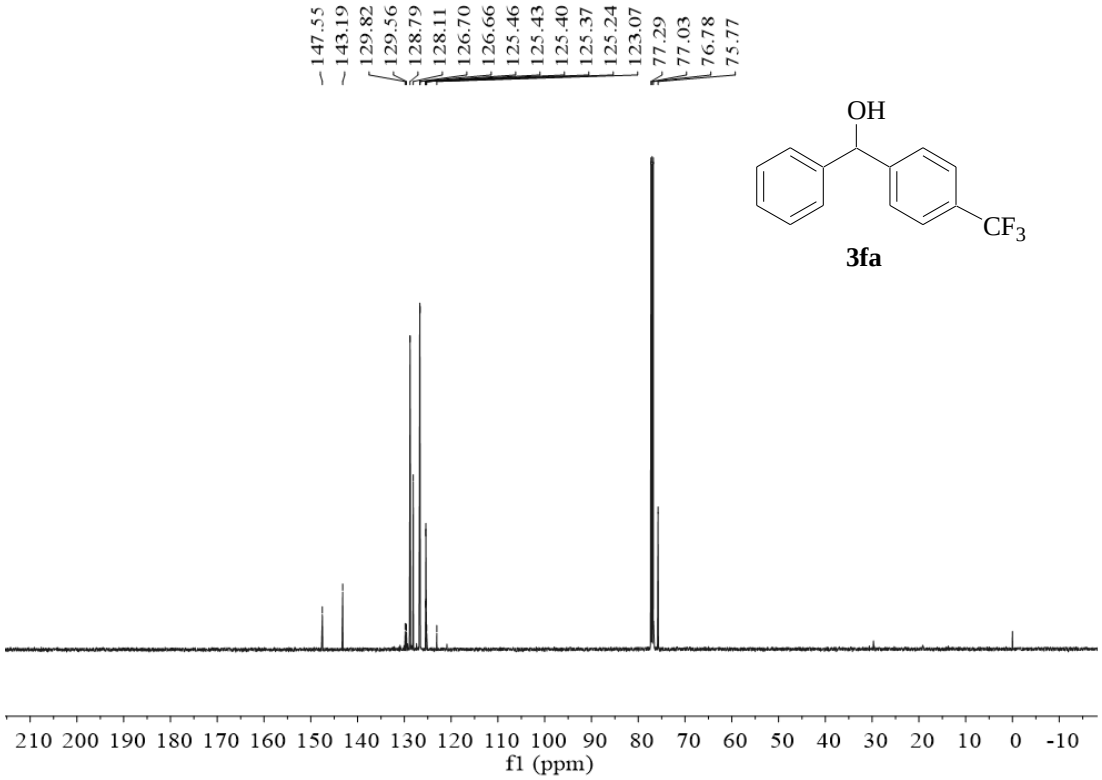
3ea

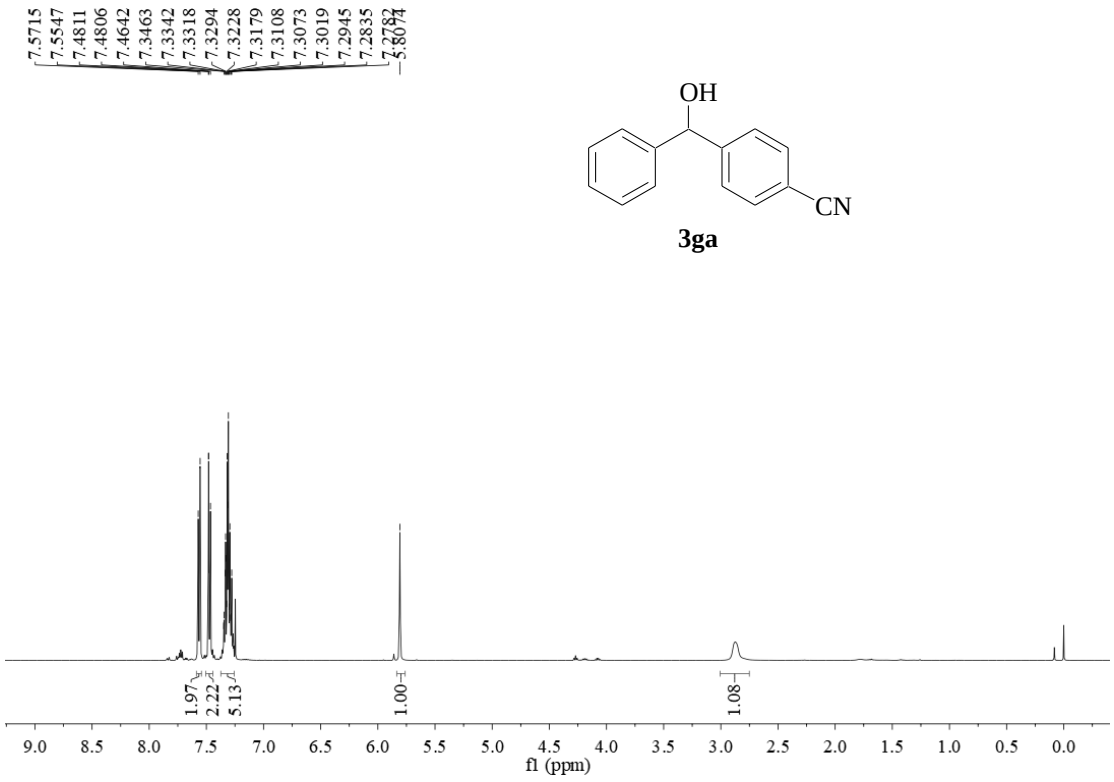

163.16
161.20
143.67
139.60
139.57
128.59
128.28
128.21
127.74
126.48
115.37
115.20
77.29
77.03
76.78
75.61
OH
F
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

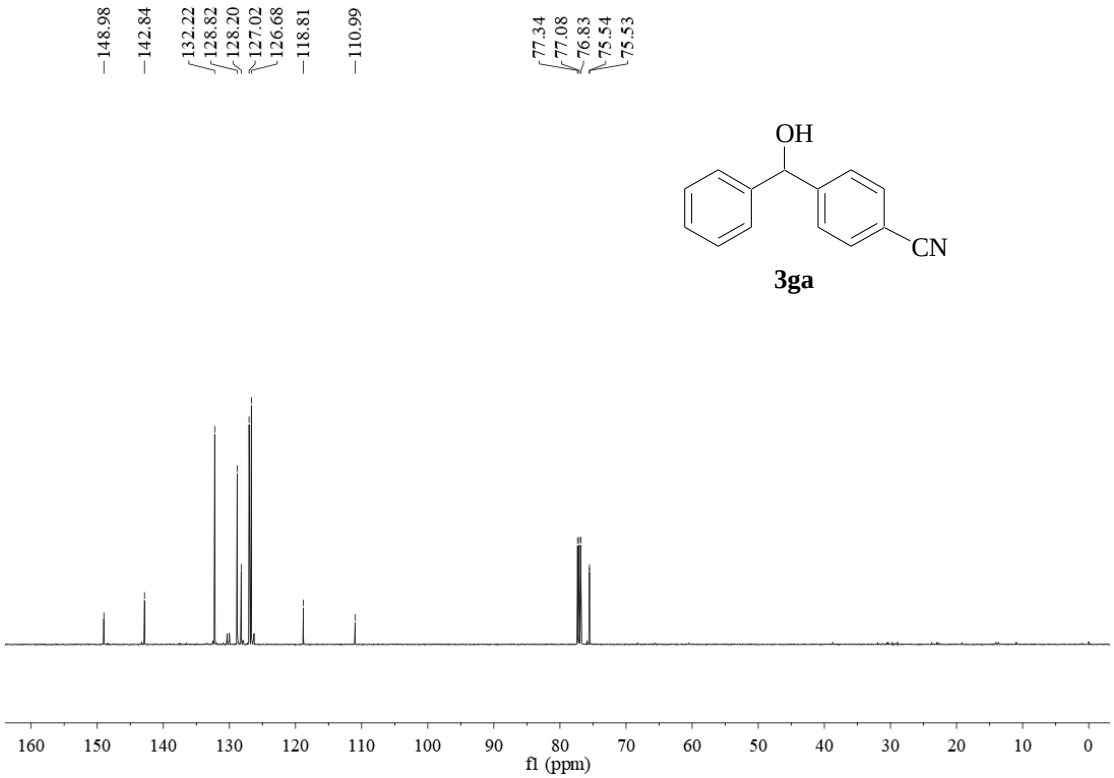
3ea


7.593
7.577
7.514
7.497
7.354
7.346
7.338
7.331
7.328
7.316
7.308
7.300
7.291
7.281
7.274
7.251
5.873
2.374
-0.000
OH
CF3
1.98
2.03
5.02
0.99
1.06
11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1.0
f1 (ppm)

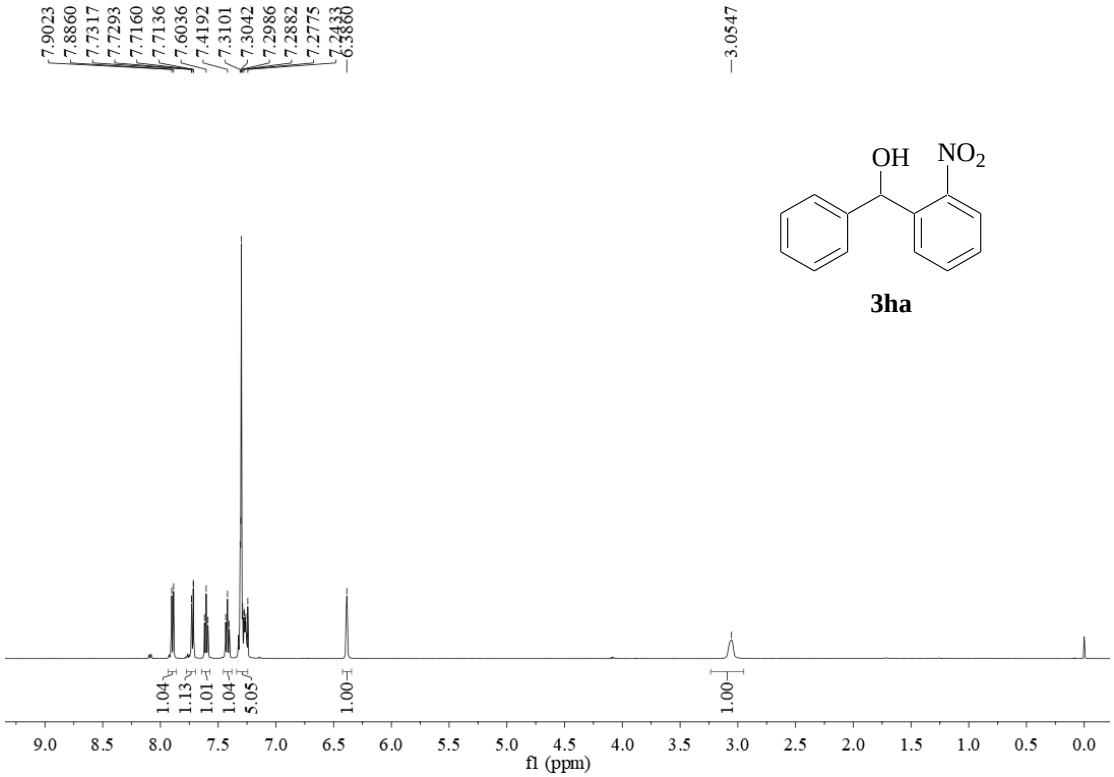
3fa


147.55
143.19
129.82
129.56
128.79
128.11
126.70
126.66
125.46
125.43
125.40
125.37
125.24
123.07
77.29
77.03
76.78
75.77
OH
CF3
3fa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.5715
7.5547
7.4811
7.4806
7.4642
7.3463
7.3342
7.3318
7.3294
7.3228
7.3179
7.3108
7.3073
7.3019
7.2945
7.2835
7.2782
5.8074
OH
CN
3ga
1.97
2.22
5.13
1.00
1.08
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


148.98
142.84
132.22
128.82
128.20
127.02
126.68
118.81
110.99
77.34
77.08
76.83
75.54
75.53
OH
CN
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3ga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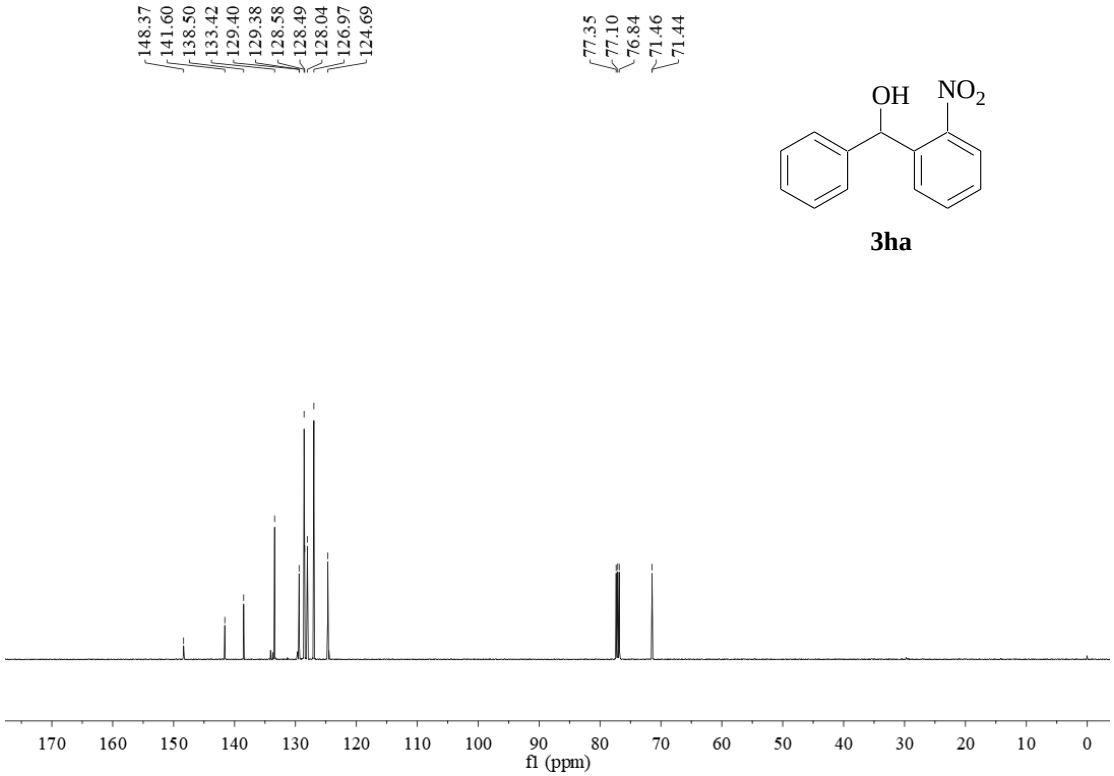
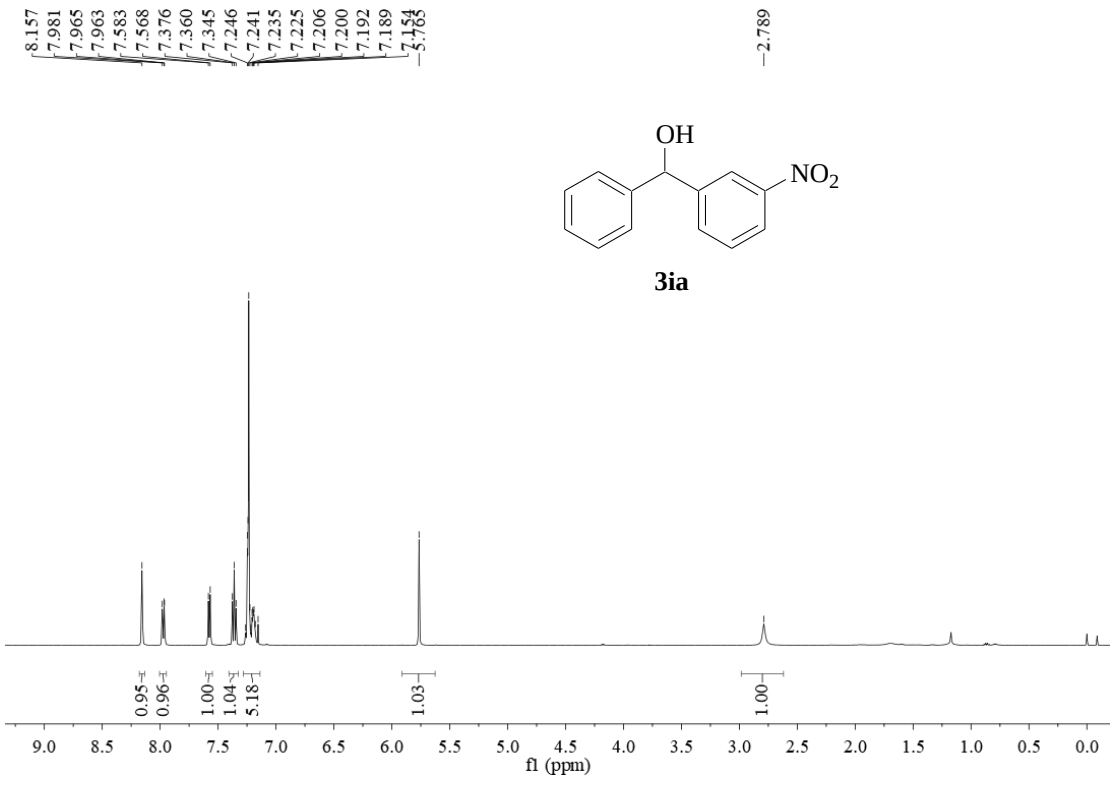
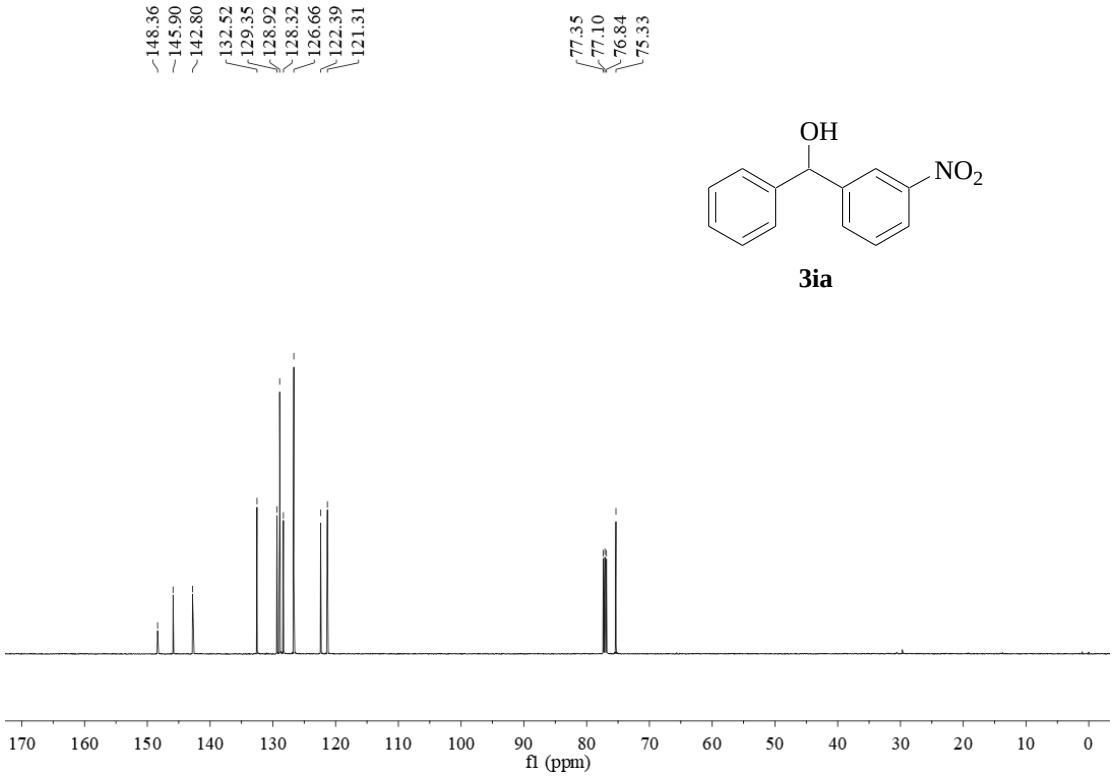
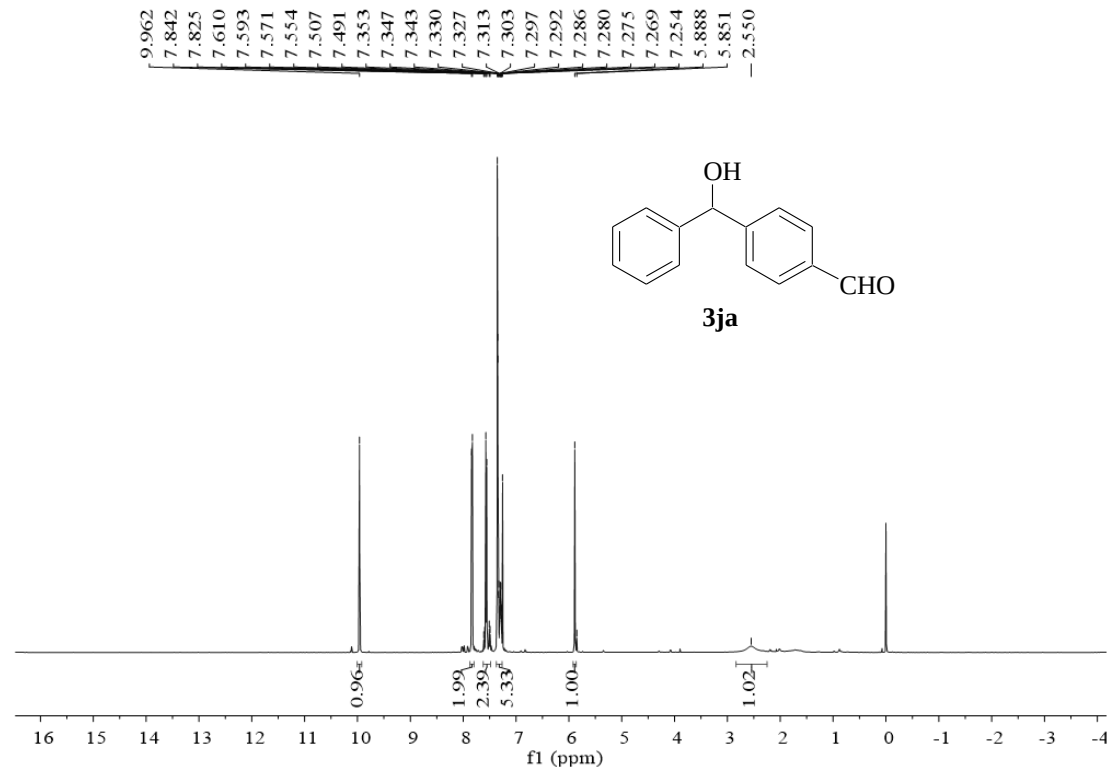
7.8860
7.7317
7.7293
7.7160
7.7136
7.6036
7.4192
7.3101
7.3042
7.2986
7.2882
7.2775
7.2433
7.2380
6.3880
3.0547
OH
NO2
1.04
1.13
1.01
1.04
5.05
1.00
1.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

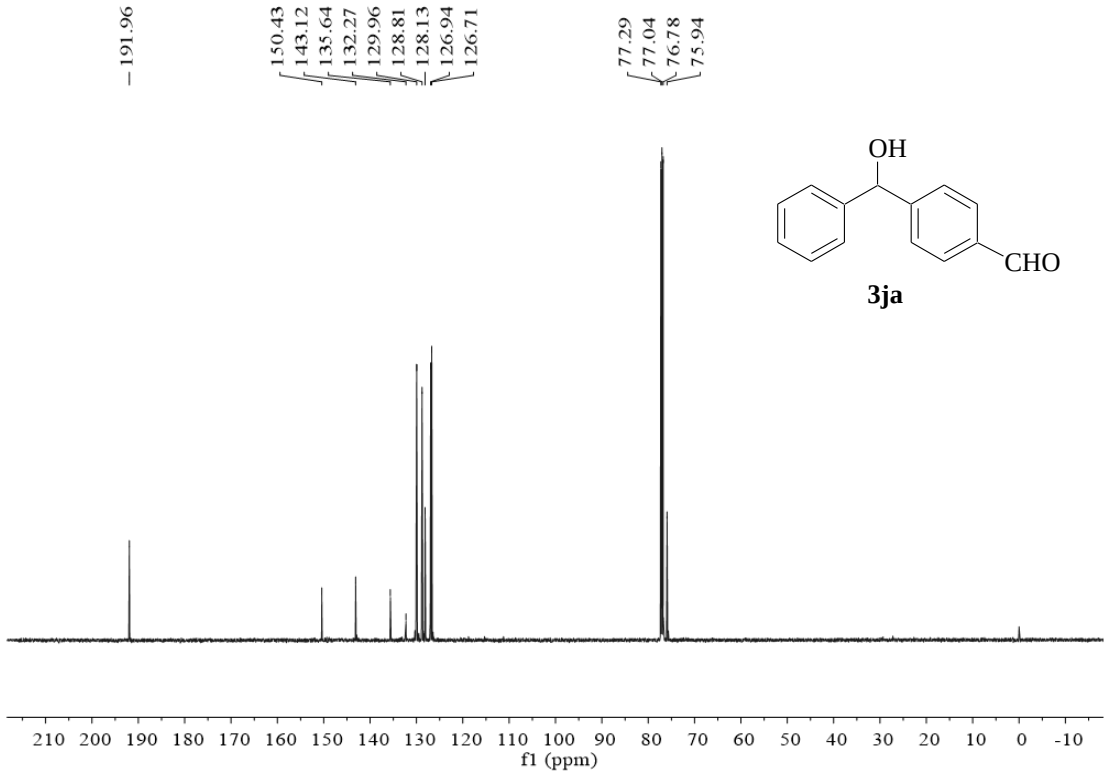
3ha

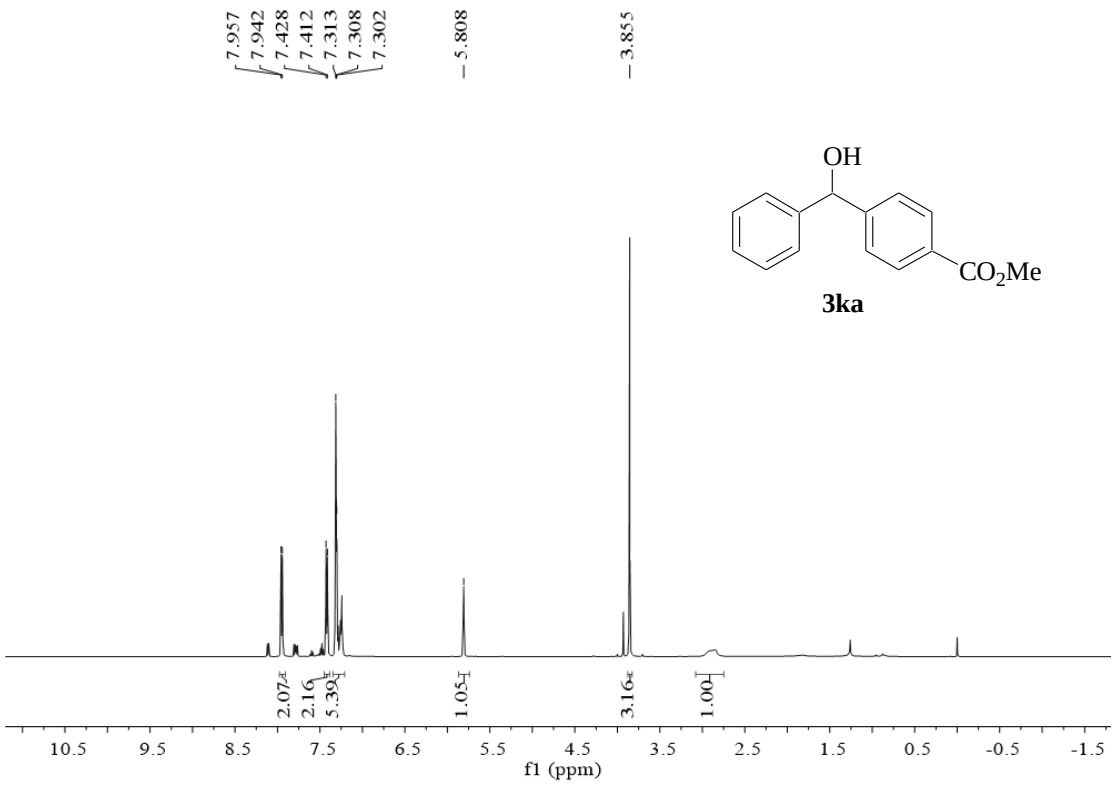

148.37
141.60
138.50
133.42
129.40
129.38
128.58
128.49
128.04
126.97
124.69
77.35
77.10
76.84
71.46
71.44
OH
NO2
3ha
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

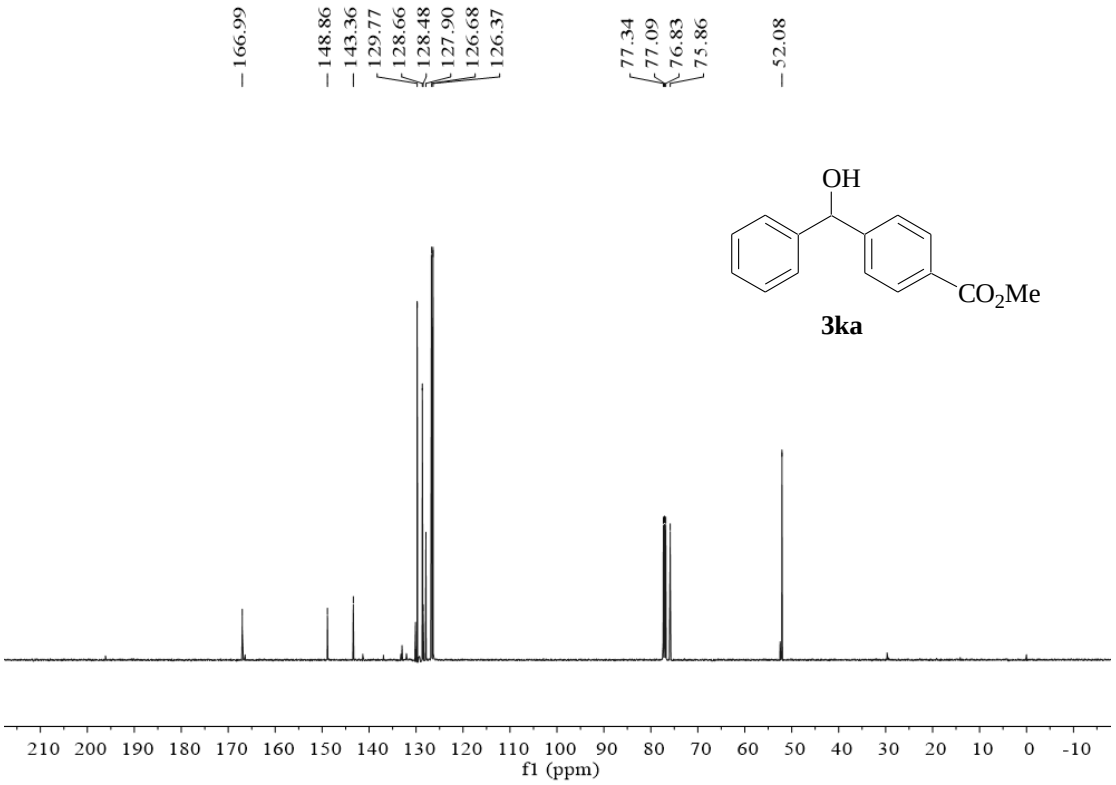

8.157
7.981
7.965
7.963
7.583
7.568
7.376
7.360
7.345
7.246
7.241
7.235
7.225
7.206
7.200
7.192
7.189
7.154
5.765
2.789
OH
NO2
3ia
0.95
0.96
1.00
1.04
5.18
1.03
1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

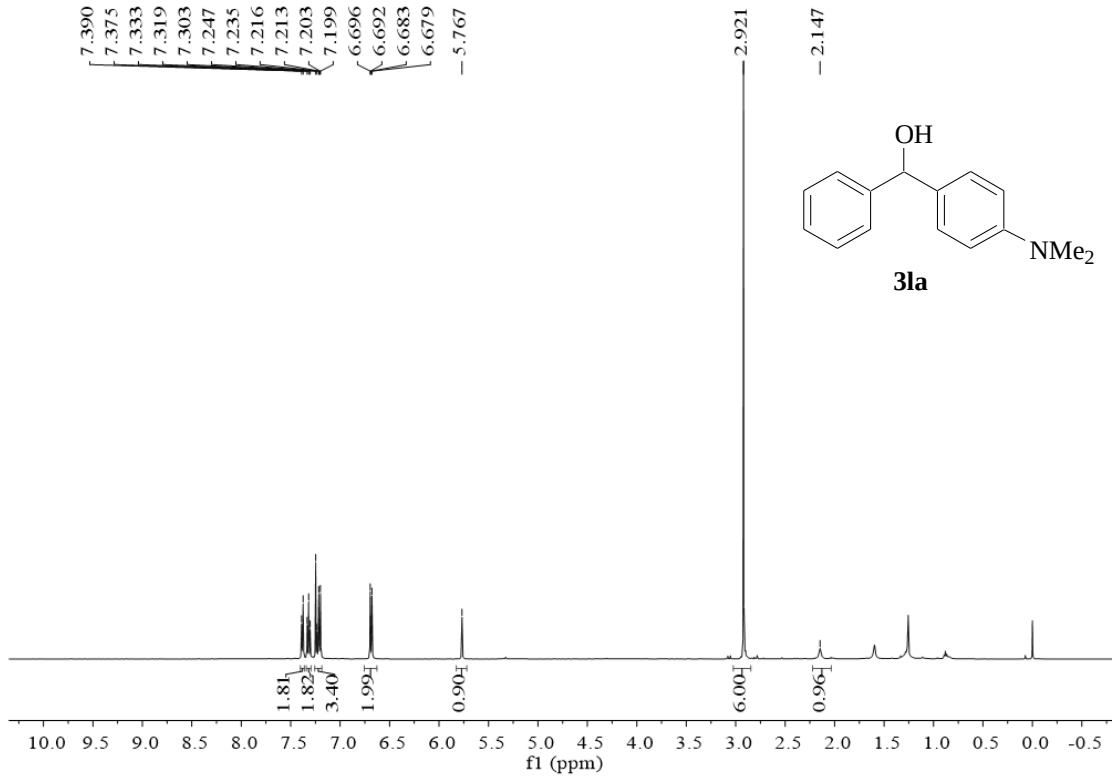

148.36
145.90
142.80
132.52
129.35
128.92
128.32
126.66
122.39
121.31
77.35
77.10
76.84
75.33
OH
NO2
3ia
f1 (ppm)

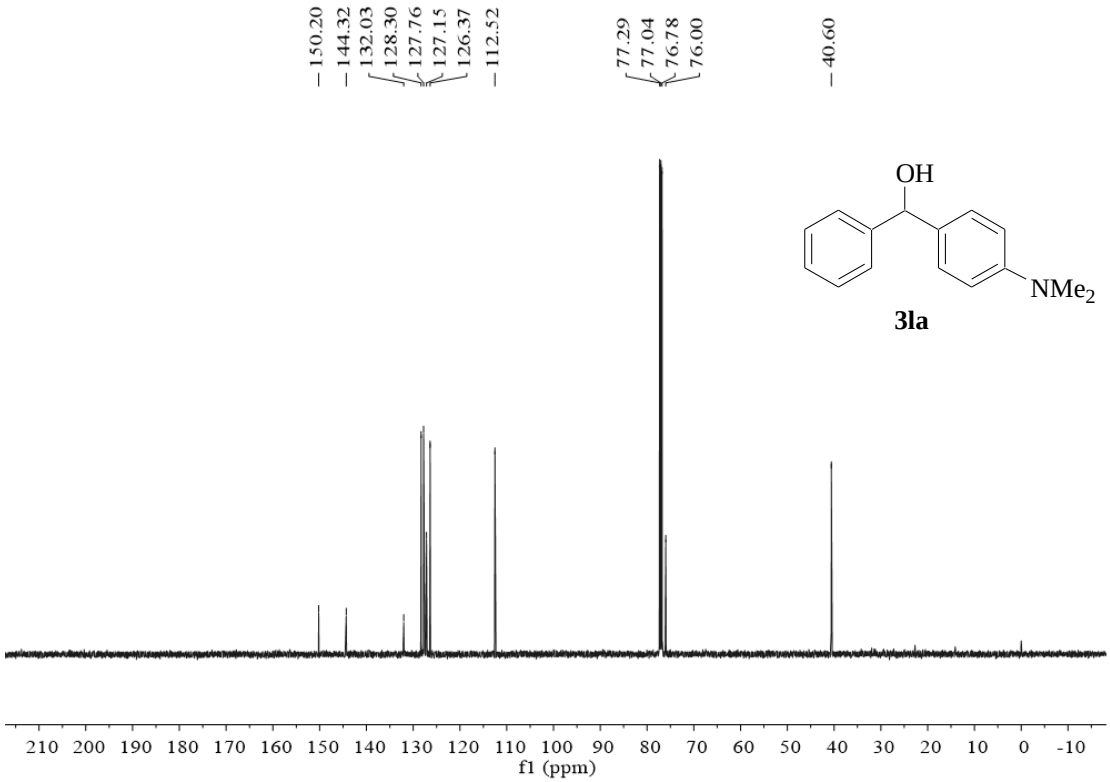

9.962
7.842
7.825
7.610
7.593
7.571
7.554
7.507
7.491
7.353
7.347
7.343
7.330
7.327
7.313
7.303
7.297
7.292
7.286
7.280
7.275
7.269
7.254
5.888
5.851
2.550
OH
CHO
3ja
0.96
1.99
2.39
5.33
1.00
1.02
f1 (ppm)


191.96
150.43
143.12
135.64
132.27
129.96
128.81
128.13
126.94
126.71
77.29
77.04
76.78
75.94
OH
CHO
3ja
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

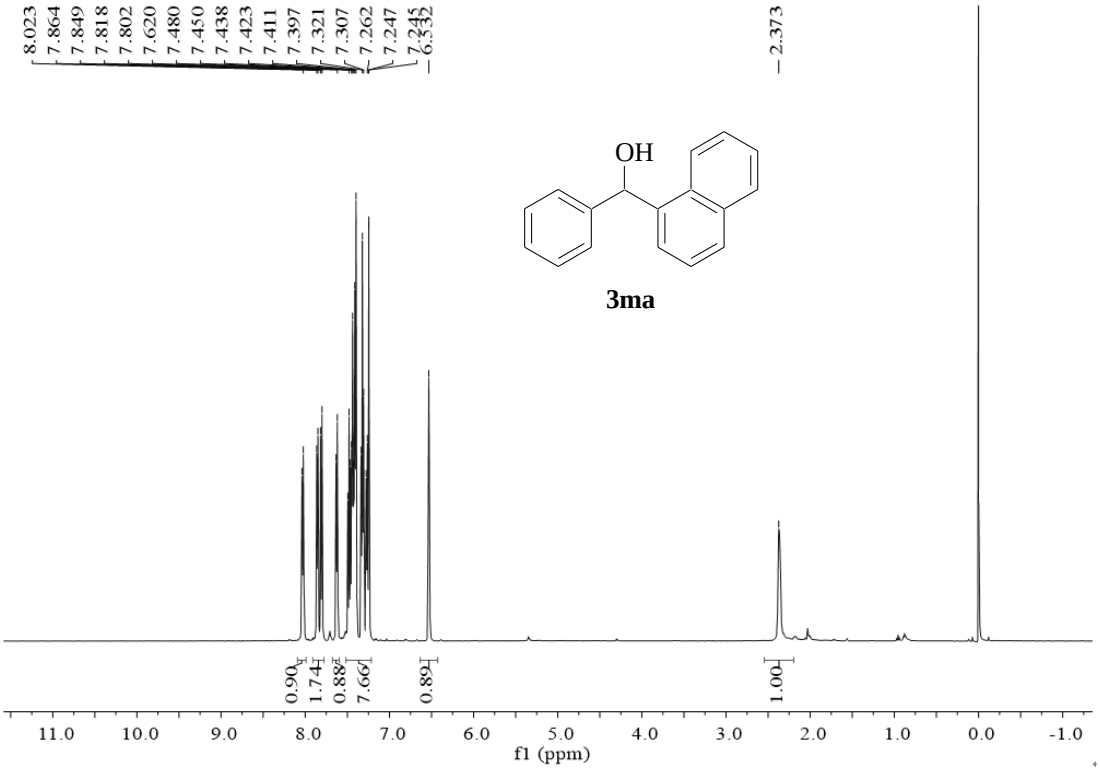

7.957
7.942
7.428
7.412
7.313
7.308
7.302
5.808
3.855
OH
CO2Me
3ka
2.07
2.16
5.39
1.05
3.16
1.00
10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0.5 -1.5
f1 (ppm)


166.99
148.86
143.36
129.77
128.66
128.48
127.90
126.68
126.37
77.34
77.09
76.83
75.86
52.08
OH
CO2Me
3ka
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

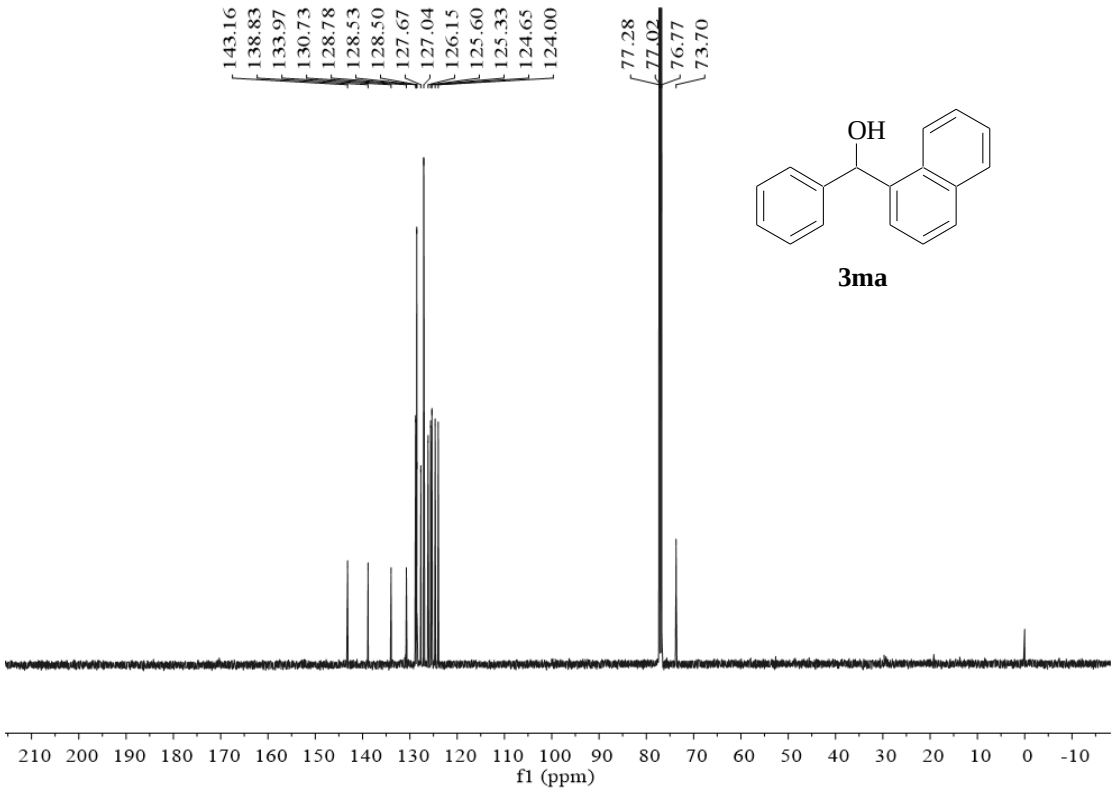

7.390
7.375
7.333
7.319
7.303
7.247
7.235
7.216
7.213
7.203
7.199
6.696
6.692
6.683
6.679
5.767
2.921
2.147
OH
NMe2
3la
1.81
1.82
3.40
1.99
0.90
6.00
0.96
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


150.20
144.32
132.03
128.30
127.76
127.15
126.37
112.52
77.29
77.04
76.78
76.00
40.60
OH
NMe2
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

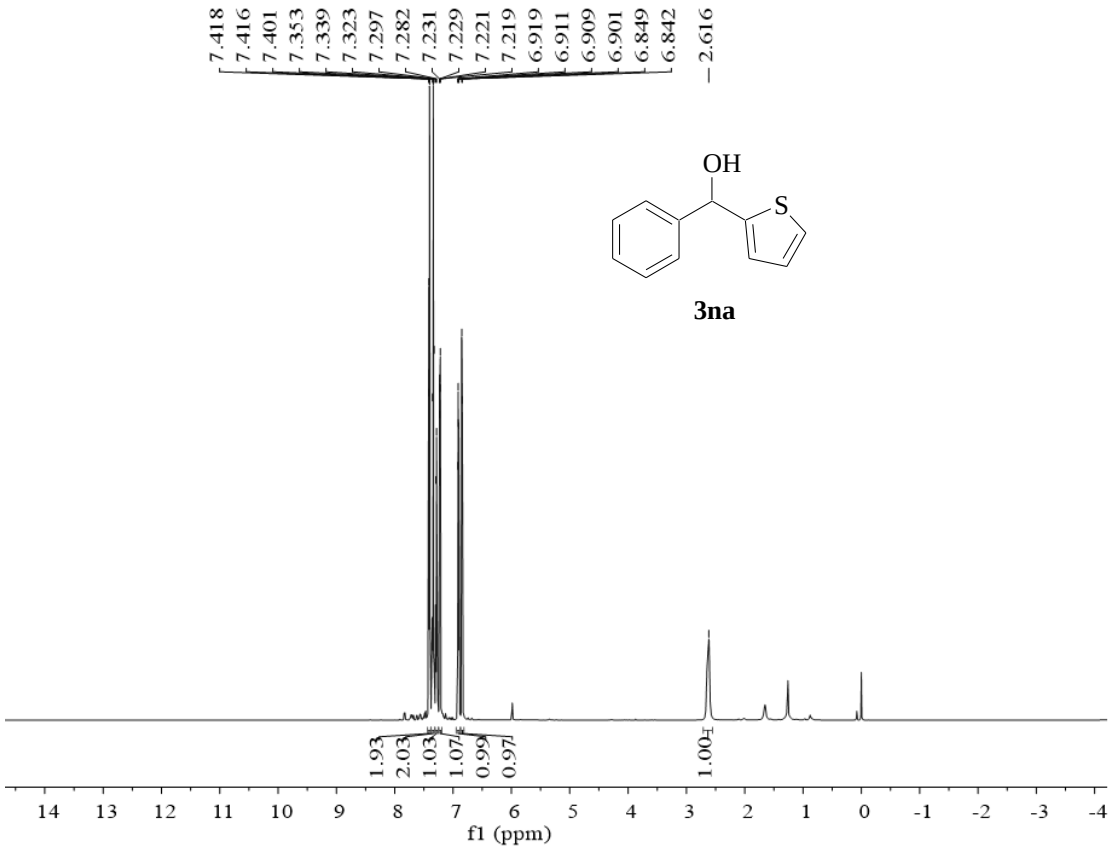
3la


8.023
7.864
7.849
7.818
7.802
7.620
7.480
7.450
7.438
7.423
7.411
7.397
7.321
7.307
7.262
7.247
7.245
6.532
2.373
OH
0.90
1.74
0.88
7.66
0.89
1.00
11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1.0
f1 (ppm)

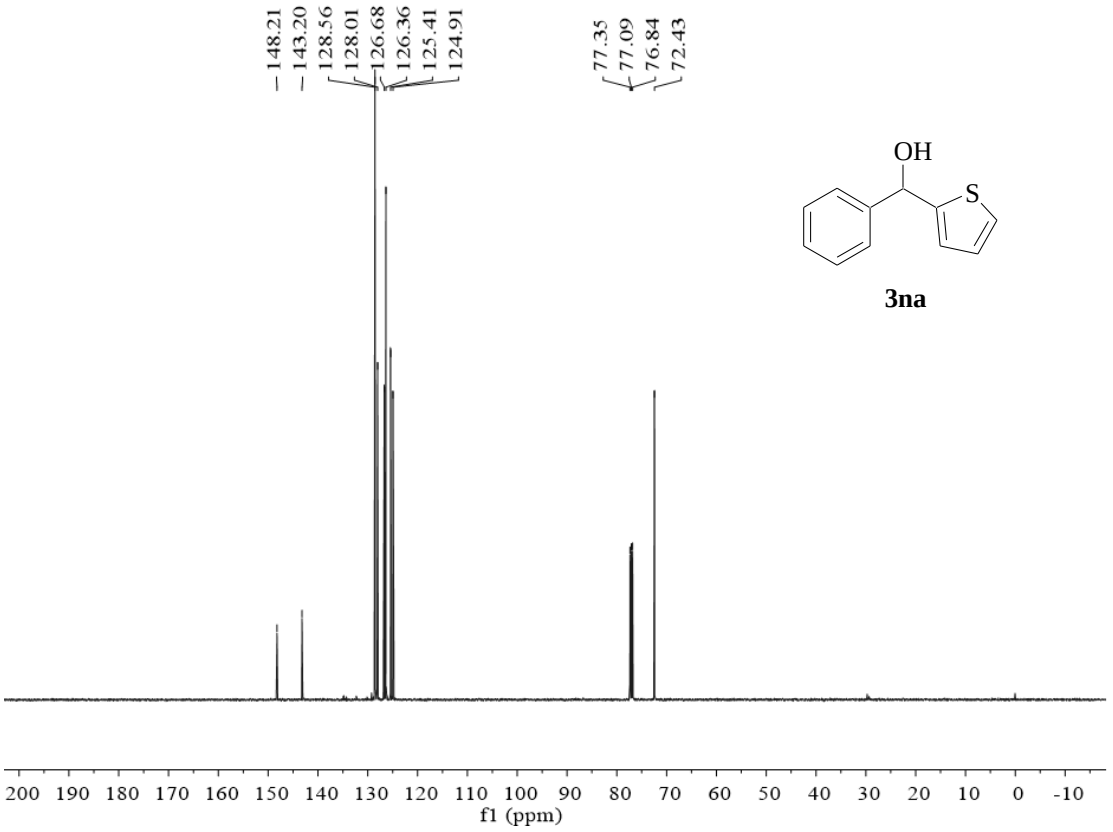
3ma


143.16
138.83
133.97
130.73
128.78
128.53
128.50
127.67
127.04
126.15
125.60
125.33
124.65
124.00
77.28
77.02
76.77
73.70
OH
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

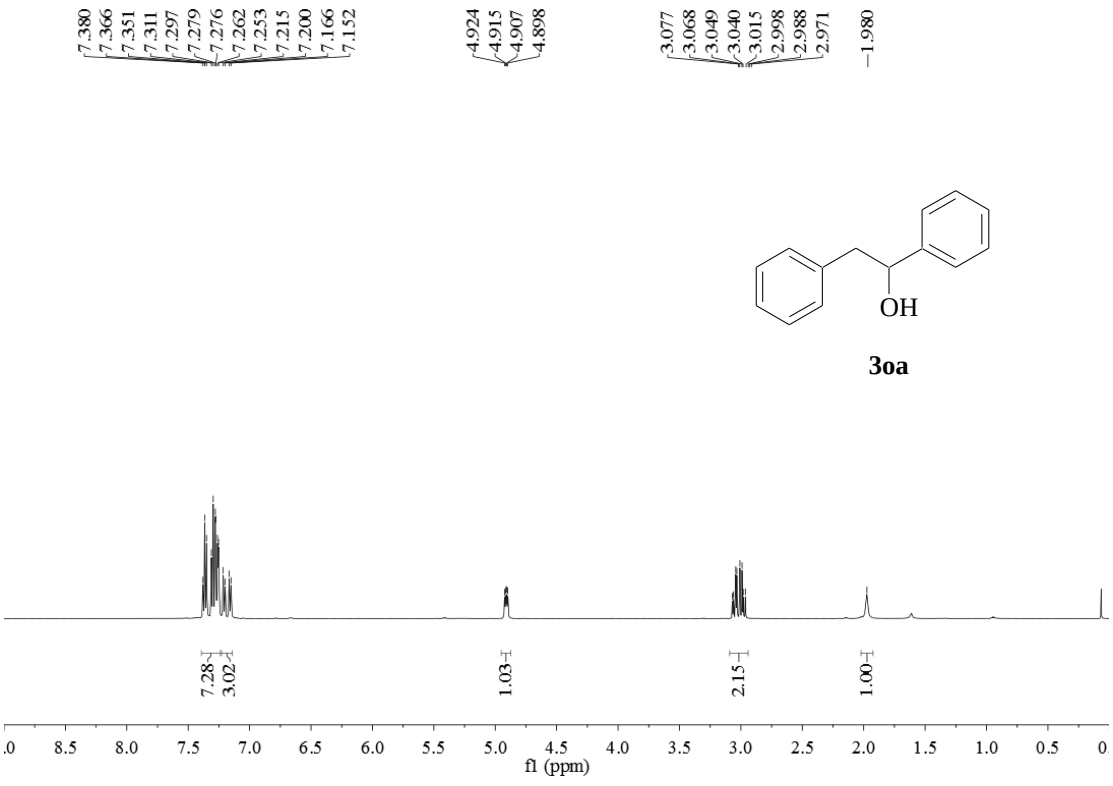
3ma


7.418
7.416
7.401
7.353
7.339
7.323
7.297
7.282
7.231
7.229
7.221
7.219
6.919
6.911
6.909
6.901
6.849
6.842
2.616
OH
S
1.93
2.03
1.03
1.07
0.99
0.97
1.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

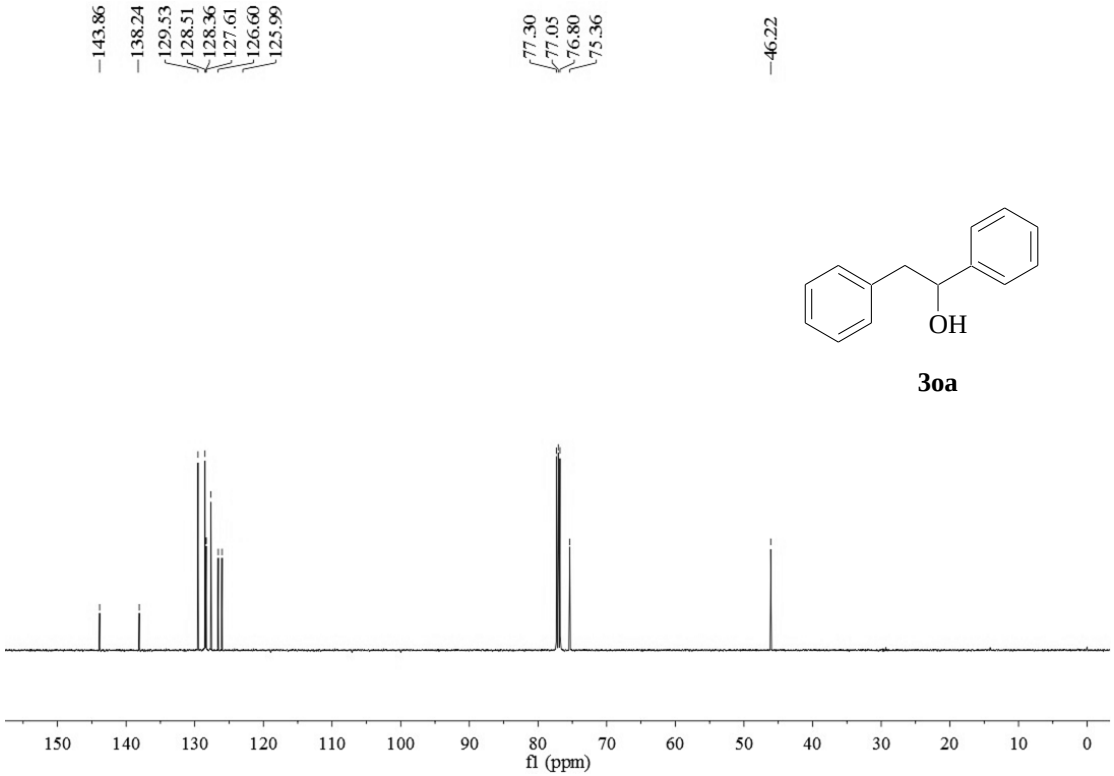
3na


148.21
143.20
128.56
128.01
126.68
126.36
125.41
124.91
77.35
77.09
76.84
72.43
OH
S
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

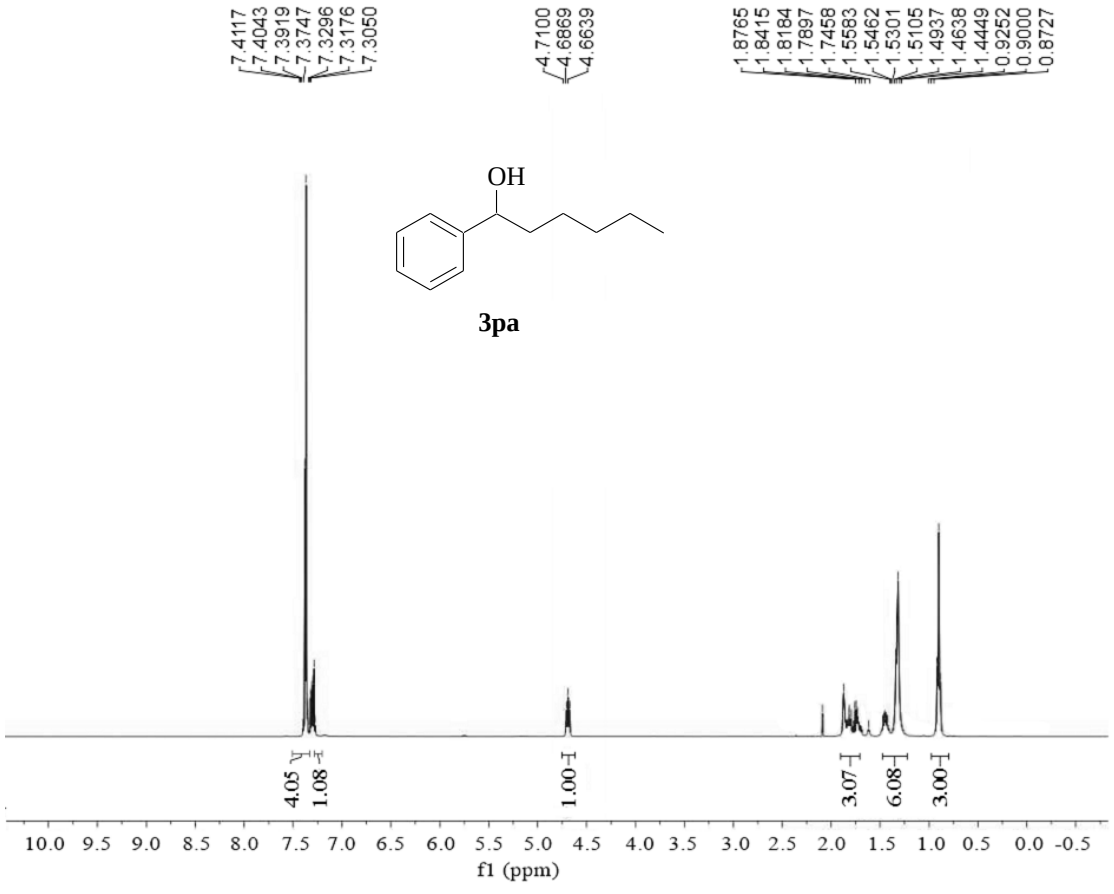
3na


7.380
7.366
7.351
7.311
7.297
7.279
7.276
7.262
7.253
7.215
7.200
7.166
7.152
4.924
4.915
4.907
4.898
3.077
3.068
3.049
3.040
3.015
2.998
2.988
2.971
1.980
OH
7.28
3.02
1.03
2.15
1.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

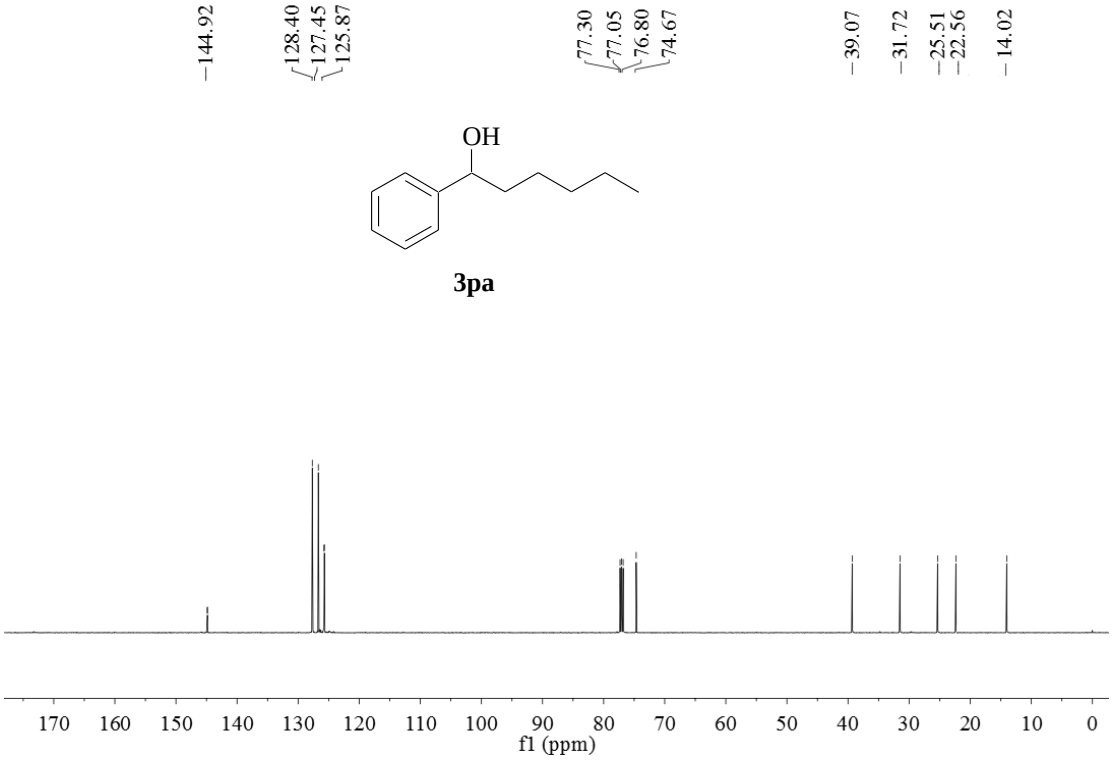
3oa


143.86
138.24
129.53
128.51
128.36
127.61
126.60
125.99
77.30
77.05
76.80
75.36
46.22
OH
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

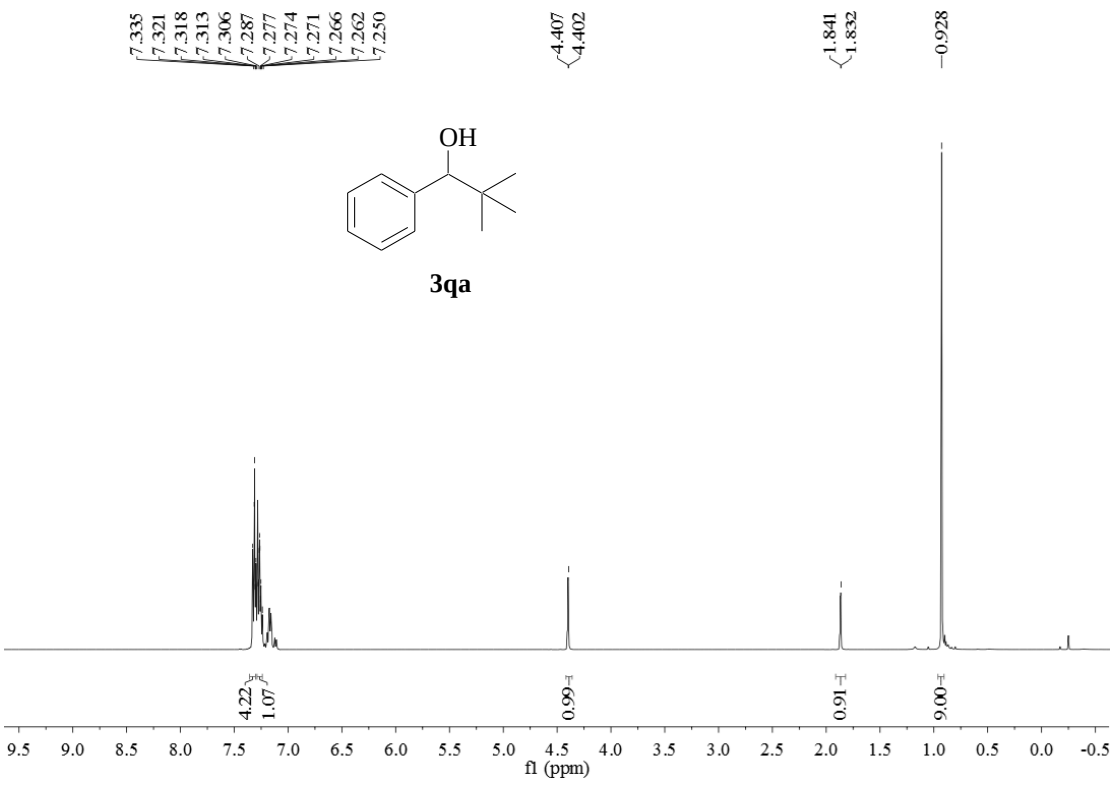
3oa


7.4117
7.4043
7.3919
7.3747
7.3296
7.3176
7.3050
4.7100
4.6869
4.6639
1.8765
1.8415
1.8184
1.7897
1.7458
1.5583
1.5462
1.5301
1.5105
1.4937
1.4638
1.4449
0.9252
0.9000
0.8727
OH
4.05
1.08
1.00
3.07
6.08
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

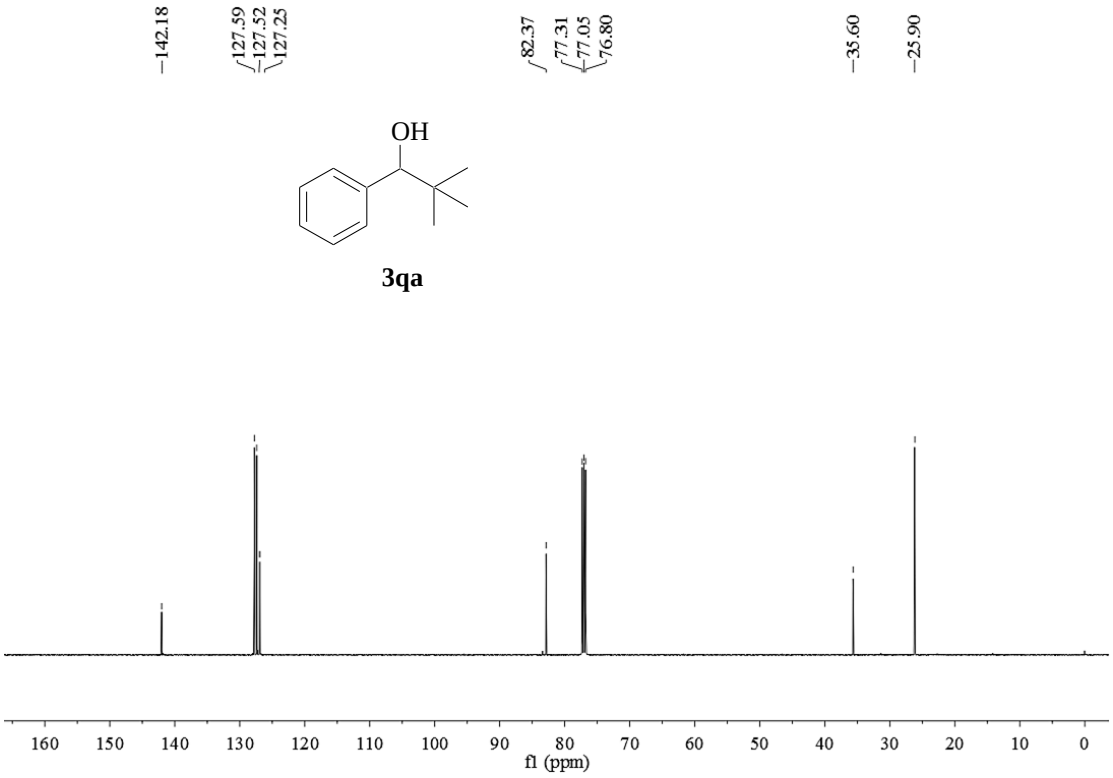
3pa


144.92
128.40
127.45
125.87
77.30
77.05
76.80
74.67
39.07
31.72
25.51
22.56
14.02
OH
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3pa


7.335
7.321
7.318
7.313
7.306
7.287
7.277
7.274
7.271
7.266
7.262
7.250
4.407
4.402
1.841
1.832
0.928
OH
4.22
1.07
0.99
0.91
9.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

3qa


142.18
127.59
127.52
127.25
82.37
77.31
77.05
76.80
35.60
25.90
OH
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

3qa